N6813618

FIREBALL AND POST-FIREBALL COMPOSITIONS AND ATMOSPHERIC CHEMISTRY OF FUEL/OXYGEN-FLUORINE PROPELLANTS

Introduction

This phase of the work carried out under NASA contract NAS10-1255 deals with the combustion products found in the fireball and combustion products cloud after a liquid propellant explosion.

This work is part of the complete study of the liquid propellant explosion characteristics carried out under the above contract. Some phases of this work have been completed others are still under way. The completion order is not quite chronological as compared with the actual phenomena as they are occurring in the liquid propellant explosions. The main reason being that some of this work is correlated with other large NASA and Air Force Projects and therefore the completion of certain parts of this work is time dependent upon these other projects.

Considerable portions of the work carried out under this contract have however been reported and are listed in the references 1,2,3,4,5,6,7 and 8.

The earlier work, part of which is still under way for the above reasons, deals with the feasibility of predicting the explosion characteristics of liquid propellants. That such predictions are feasible was reported upon in (1). This reference presented a method of obtaining the yield without going into detail of the involved phenomena. It gives the results expected and needed.

References 4,5,6,7, and 8 look into the details and characteristics of the processes involved, leading to the results which are to be predicted.

The complete problem is divided into three distinctive parts

A. Chemical Kinetics & Heat Transfer

B. Fluid Hydrodynamics & Heat Transfer

C. Combustion and Detonation Initiation and Propagation

In other words, depending upon the type of propellants present and the mode of failure involved the maximum possible yield obtainable (yield potential) can be determined (6). This is if the propellants are mixed as well as can be and the result is purely theoretical.

Since the mixing of the fluids is governed by the hydrodynamic laws and since we have fluids at different temperatures also by the fundamentals of heat transfer, the amount of the propellants mixed at any time can be determined (6,7).

The magnitude of the explosion yield which could be obtained at any time is the portion mixed times the theoretical maximum. This is because only the portion of the propellants mixed at the time of detonation can take part in this process (6).

Having thus obtained from A and B the expected yield at any time, to determine what the actual yield will be, it is necessary to know at what time during the processes detonation will occur. The determination of this critical time is the problem of part C.

Studies are now under way which deal with each of the separate and distinct phenomena and then when enough of the information is available combining the results of the three parts should give the actual yield (6).

After the detonation has occurred the behavior of the fireball from the explosion which is formed and then gradually changes into a combustion products cloud is of importance. How large a fireball is formed, what is its temperature and what are the pressures inside? To be able to obtain this information the knowledge of how the fireball comes about, how it cools and then changes into a combustion products cloud is essential. Thus, its behavior is really one of the last groups of phenomena or processes in a series.

So, for this phase of the work the knowledge of the fireball and combustion cloud, volume-time, pressure-time and temperature-time histories have been assumed known and then the composition of the combustion phenomena has been determined. The composition of the fireball and of the combustion cloud are important as well as their interaction with the atmosphere especially when toxic materials such as Fluorine are used in the propellants.

The volume-time, pressure-time, and temperature-time histories of the explosion from liquid propellants were chosen as the input since they may be determined theoretically or may be measured in experiments thus giving a check on the theoretically determined information, with statistical variations, etc.

For this report the best information available at this time has been used as the input and then rather elaborate computer programs have been used in obtaining the desired results. Homogeneity of the fireball and of the combustion products cloud have been assumed in all calculations and this seems to be a reasonably good basis since the turbulence of the reaction processes is great enough to tend to mix the different products well.

Theory of Approach

Equilibrium Composition of Chemical Reactions of Liquid Propellants Taking Place in the Atmosphere.

The purpose of this phase of the research program is to theoretically determine the amounts of product gases formed, as a function of time, as the result of a reaction involving liquid propellants and entrained air. This type of reaction is continuous since all of the available fuel does not react immediately and furthermore the resulting fireball (which grows with time as more fuel reacts) continually entrains air. Given the initial amounts of fuel and oxidant as well as the volume - time history of the fireball (theoretically determined or as observed from high speed films), equilibrium compositions can be determined.

The equilibrium composition for the system of n products of reaction is determined by the simultaneous solution of $n+1$ equations consisting of the equations of mass balance, pressure balance and the dissociation equations involving equilibrium constants.

Assuming a constant pressure process as well as an instantaneous reaction time and making use of either theoretically obtained or experimentally determined pressure-time and temperature-time histories of the fireball, a solution is found such that the total theoretical volume of the products of reaction is made identically equal to the total experimental volume by adjusting the fuel burning rate and/or adjusting the amount of entrained air. As a first approximation, it is further assumed that no air entrainment exists until all of the available fuel is burned.

To efficiently meet these demands, a computer program has been developed. The program is general but limited here to the following reactants: liquid hydrogen, kerosene (RP-1), liquid oxygen, liquid fluorine, and air. Fifteen products of reaction were considered.

The equations and method of solution follows.

Controlling Equations:

Symbol	Description	Reactant
A_1	moles of LH_2	A_1H_2
A_2	moles of RP-1	$A_2C_xH_{2x}$
A_3	moles of LO_2	A_3O_2
A_4	moles of LF_2	A_4F_2
A_5	moles of air	$\frac{A_5}{4.79}(O_2 + 3.79\ N_2)$

The reactants can then be written as:

$$(A_1 + A_2X)\ H_2 + (A_3 + 0.209A_5)\ O_2 + A_4F_2 + 0.792A_5N_2 + A_2XC$$

Consider the following products of reaction; such that the right hand side of the equilibrium equation is

$$\frac{N}{P}\ (p_1H_2O + p_2CO_2 + p_3H_2 + p_4N_2 + p_5F_2 + p_6O_2 + p_7HF + p_8CO$$
$$+ p_9NO + p_{10}OH + p_{11}H + p_{12}N + p_{13}F + p_{14}C + p_{15}O)$$

where,

N = total number of moles of products of reaction

P = total pressure

p_i = partial pressure of i^{th} product

The unknowns are p_i ($i = 1, \ldots 15$), N. Hence 16 equations are necessary for a solution. The balance equations are:

(a) Pressure Balance

$$P - \sum p_i = 0$$

(b) Hydrogen Balance

$$2(A_1 + A_2X) - \frac{N}{P}\ (2p_1 + 2p_3 + p_7 + p_{10} + p_{11}) = 0$$

(c) Oxygen Balance

$$2(A_3 + 0.209A_5) - \frac{N}{P}(p_1 + 2p_2 + 2p_6 + p_8 + p_9 + p_{10} + p_{15}) = 0$$

(d) Nitrogen Balance

$$1.584\, A_5 - \frac{N}{P}(2p_4 + p_9 + p_{12}) = 0$$

(e) Carbon Balance

$$A_2X - \frac{N}{P}(p_2 + p_8 + p_{14}) = 0$$

(f) Flucrine Balance

$$2A_4 - \frac{N}{P}(2p_5 + p_7 + p_{13}) = 0$$

The above 6 equations can be reduced to 5 equations by eliminating $\frac{N}{P}$. Since we will be dealing with hydrogen (either LH_2 and / or RP-1), $\frac{N}{P}$ can be eliminated by dividing the 2nd equation into the last 4 equations. The 5 equations are:

$$P - p_1 - p_2 - \cdots\cdots - p_{15} = 0 \tag{1}$$

$$(2Y_1 - Y_2)\, p_1 - 2Y_2p_2 + 2Y_1p_3 - 2Y_2p_6 + Y_1p_7 - Y_2p_8 - Y_2p_9 + (Y_1 - Y_2)\, p_{10} + Y_1p_{11} - Y_2p_{15} = 0 \tag{2}$$

$$2Y_3p_1 + 2Y_3p_3 - 2Y_2p_4 + Y_3p_7 - Y_2p_9 + Y_3p_{10} + Y_3p_{11} - Y_2p_{12} = 0 \quad (3)$$

$$2Y_4p_1 - Y_2p_2 + 2Y_4p_3 + Y_4p_7 - Y_2p_8 + Y_4p_{10} + Y_4p_{11} - Y_2p_{14} = 0 \quad (4)$$

$$2Y_5p_1 + 2Y_5p_3 - 2Y_2p_5 + (Y_5 - Y_2)p_7 + Y_5p_{10} + Y_5p_{11} - Y_2p_{13} = 0 \quad (5)$$

where

$$Y_1 = 2(A_3 + 0.209A_5)$$

$$Y_2 = 2(A_1 + A_2X)$$

$$Y_3 = 1.584A_5$$

$$Y_4 = A_2X$$

$$Y_5 = 2A_4$$

The remaining 10 equations required for a solution are the dissociation equations. Tables of equilibrium coefficients are available (20) in terms of partial pressures rather than concentrations of the products of reaction. The appropriate equations are given below.

$2H + O \rightarrow H_2O$	such that	$p_1 - K_1 p_{11}^2 p_{15} = 0$	(6)
$C + 2O \rightarrow CO_2$	such that	$p_2 - K_2 p_{14} p_{15}^2 = 0$	(7)
$2H \rightarrow H_2$	such that	$p_3 - K_3 p_{11}^2 = 0$	(8)
$2N \rightarrow N_2$	such that	$p_4 - K_4 p_{12}^2 = 0$	(9)
$2F \rightarrow F_2$	such that	$p_5 - K_5 p_{13}^2 = 0$	(10)
$2O \rightarrow O_2$	such that	$p_6 - K_6 p_{15}^2 = 0$	(11)
$H + F \rightarrow HF$	such that	$p_7 - K_7 p_{11} p_{13} = 0$	(12)
$C + O \rightarrow CO$	such that	$p_8 - K_8 p_{14} p_{15} = 0$	(13)
$N + O \rightarrow NO$	such that	$p_9 - K_9 p_{12} p_{15} = 0$	(14)
$O + H \rightarrow OH$	such that	$p_{10} - K_{10} p_{11} p_{15} = 0$	(15)

The equilibrium coefficients K_i vary systematically with the temperature of the reaction. It is assumed that the products of reaction calculated at a particular temperature and pressure, are formed instantaneously. Hence, one need only solve the above 15 equations for given values of P, T, and the amounts of reactants, to arrive at the equilibrium composition.

Solution of These Equations:

Since the dissociation equations are non-linear, there exists no direct solution. The Newton-Raphson method is used to obtain a "trial and error" solution.

(1) Initially, estimates of p_i $(i = 1, .., 15)$ are taken and each of the 15 equations is expanded in a Taylor's series about the estimated point, p_i.

(2) Corrections to p_i are then found (Δp_i) and the new estimates of p_i, given by $p_i + \Delta p_i$, are used in place of the initial estimates in (1).

(3) The procedure is repeated until Δp_i becomes negligible.

Consider a solution to two non-linear equations; $f(x,y) = 0$, $g(x,y) = 0$.

Let the initial estimate of the required solution (x,y) be the point $x_1,y_1)$. Expanding f, g in a Taylor's series about the point (x_1,y_1), then

$$f(x,y) = 0 = f(x_1,y_1) + \frac{\partial f}{\partial x}(x_1,y_1).(x-x_1) + \frac{\partial f}{\partial y}(x_1,y_1).(y-y_1) + \ldots\ldots$$

$$g(x,y) = 0 = g(x_1,y_1) + \frac{\partial g}{\partial x}(x_1,y_1).(x-x_1) + \frac{\partial g}{\partial y}(x_1,y_1)\cdot(y-y_1) + \ldots\ldots$$

or

$$\Delta f = \frac{\partial f}{\partial x}.\Delta x + \frac{\partial f}{\partial y}.\Delta y + \ldots$$

$$\Delta g = \frac{\partial g}{\partial x}.\Delta x + \frac{\partial g}{\partial y}.\Delta y + \ldots$$

where

$$\Delta f = f(x,y) - f(x_1,y_1) = - f(x_1,y_1)$$

$$\Delta g = g(x,y) - g(x_1,y_1) = - g(x_1,y_1)$$

and

$$\Delta x = x-x_1$$

$$\Delta y = y-y_1$$

Hence the non-linear equations have been transformed into linear correction equations of the form

$$f(x_1,y_1) + f_x .\Delta x + f_y .\Delta y = 0$$

$$g(x_1,y_1) + g_x .\Delta x + g_y .\Delta y = 0$$

where $f_x = \frac{\partial f}{\partial x}$, $f_y = \frac{\partial f}{\partial y}$, etc., and the derivatives of second order and higher have been neglected.

The equations are solved for Δx, Δy and new estimates are given by $x_1 + \Delta x$, $y_1 + \Delta y$. The procedure is repeated until the desired accuracy is obtained.

The full procedure can best be demonstrated with an example.

<u>Example</u>:

Consider a solution to

$$f(x,y) = x^2y + y^2 + 3 = 0$$
$$g(x,y) = x^3 - 2xy^2 + 4y = 0$$

then

$$f_x = 2xy$$
$$f_y = x^2 + 2y$$
$$g_x = 3x^2 - 2y^2$$
$$g_y = -4xy + 4 = 4(1 - xy)$$

Let $x_1 = 1$, $y_1 = -1$, be the initial estimates.

Then substituting into the linear correction equations

$$3 - 2\Delta x - \Delta y = 0$$
$$-5 + \Delta x + 8\Delta y = 0$$

the solution to the above equations is

$$\Delta x = 38/30 \simeq 1.3$$
$$\Delta y = 7/15 \simeq 0.5$$

The new estimates of x, y are given by x_2, y_2 where

$$x_2 = x_1 + \Delta x = 2.3$$
$$y_2 = y_1 + \Delta y = -0.5$$

Substituting into the linear correction equations, then

$$0.6 - 2.5\Delta x + 4.3\Delta y = 0$$
$$9 + 15.4\Delta x + 10\Delta y = 0$$

The solution to the above equations is

$$\Delta x \simeq -0.4$$
$$\Delta y \simeq -0.3$$

The new estimates for x, y become

$$x_2 + \Delta x = 1.9$$
$$y_2 + \Delta y = -0.8 \qquad \text{etc.}$$

The correct solution is $(2, -1)$.

For more than 2 unknowns, the linear correction equations take the form

$$f(x,y,z,\ldots) + f_x \cdot \Delta x + f_y \cdot \Delta y + f_z \cdot \Delta z + \ldots\ldots = 0$$

$$g(x,y,z,\ldots) + g_x \cdot \Delta x + g_y \cdot \Delta y + g_z \cdot \Delta z + \ldots\ldots = 0$$

$$h(x,y,z,\ldots) + h_x \cdot \Delta x + h_y \cdot \Delta y + h_z \cdot \Delta z + \ldots\ldots = 0$$

$$i(x,y,z,\ldots) + \ldots\ldots = 0$$

$$j(x,y,z,\ldots) + \ldots\ldots$$

etc.

where the subscripted variable, f_x for example, represents the partial derivative of $f(x,y,z,\ldots)$ with respect to x.

Denoting equations (1) to (15) by B_i ($i = 1, \ldots, 15$); the correction equations are given by

$$B_1 + A_{1,1} \cdot \Delta p_1 + A_{1,2} \cdot \Delta p_2 + \ldots + A_{1,15} \cdot \Delta p_{15} = 0$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$B_{15} + A_{15,1} \cdot \Delta p_1 + A_{15,2} \cdot \Delta p_2 + \ldots + A_{15,15} \cdot \Delta p_{15} = 0$$

where $A_{i,j}$ is the partial derivative of B_i with respect to p_j. For example, $A_{7,14}$ is the partial derivative of equation (7), i.e. B_7, with respect to p_{14}. The equations are solved for Δp_i (i = 1 to 15) by first assuming initial estimates of p_i. Subsequent estimates of p_i are given by $p_i + \Delta p_i$ and the procedure is repeated until Δp_i approaches zero.

The coefficients of the correction equations $(A_{i,j})$ are denoted by matrix A and the constants B_i are denoted by the vector, -B. Hence, in matrix notation, the set of linear correction equations is given by

$$B = A \, . \Delta p$$

and its solution is given by

$$\Delta p = A^{-1} B$$

where A^{-1} is the inverse matrix.

Outline for the Fortran IV Computer Program

The program is presently designed to handle nine sets of values of pressure, temperature and volume for a given propellant mixture. That is, equilibrium coefficients are incorporated into the program for values of temperature between 3000 K and 1400 K in 200 degree increments.

Input data:

The following information is required:

(a) Weights of reactants, i.e., the total amount of fuel and oxidizer available.

(b) Yield

(c) Temperature of reaction

(d) Pressure at which reaction occurs

(e) Volume of products of reaction

Assumptions:

The following assumptions are implied:

(a) Constant pressure process

(b) Instantaneous reaction time

(c) No air entrainment until all of the available propellants are used up

Procedure

For each data point (i.e. for a given value of P, T, and V) the program determines the partial pressures of the products of reaction such that the theoretical volume of the product gases is identical to the given input volume.

For the first data point, however, since no value of volume is available, the yield is used to determine the initial amounts of propellant burned and the partial pressures are then determined.

For subsequent data points, the fuel burning rate is continually adjusted and partial pressures are calculated in turn so that finally the resultant theoretical volume becomes identical to the given (theoretically determined or experimentally evaluated) volume.

This latter procedure is repeated for subsequent data points until all of the available fuel is used up. From then on, air is added as a reactant combined with all of the available fuel in order to satisfy the "identical volume" condition.

The program also converts the resultant partial pressures into the following:

1. Pound Moles
2. Pressure-Ratios, Mole-Ratios, Volume-Ratios
3. Pound Weights
4. Weight-Ratios

The fuel burning rate, the amount of entrained air, and the theoretical volume for each data point are also determined.

Subroutine Invert

The subroutine solves the set of linear equations

$$\Delta p = A^{-1} B$$

The input data card is

CALL INVERT (A, NA, NAD, B, NB, NBD, DETERM, IERROR)

where
- A = matrix of order NA
- B = vector having NB-1 constant vector
- NAD = row dimension of A in main program
- NBD = row dimension of B in main program
- DETERM = dummy
- IERROR = dummy

The output consists of A^{-1} placed in A, Δp placed in B, and the determinant of A placed in DETERM. IERROR is an error signal equal to 0 for successful inversion; equal to -1 for overflow, equal to +1 if no inverse is obtainable.

The maximum size of A can be 100 x 100.

Symbols Used in Main Program

Subscripted Variables:

A - coefficients appearing in the correction equations

B - constant appearing in the correction equations

C - equilibrium constants

P - partial pressure

PR - partial pressure-ratio, mole-ratio, volume-ratio

PT - total pressure

T - temperature

TNT - partial moles

V - volume

WMOL - molecular weight

WT - partial weight

WTR - partial weight-ratio

Floating point variables:

F2 - weight of liquid fluorine available

H2 - weight of liquid hydrogen available

O2 - weight of liquid oxygen available

RP1 - weight of liquid RP-1 available

RNAIR - mole-ratio of entrained air

RWAIR - weight-ratio of entrained air

TN - total theoretical moles of products of reaction

TNE - total experimental moles of products of reaction

TVOL - total theoretical volume of products of reaction

WAIR - weight of entrained air

X - number of carbon atoms in the RP-1 molecule, C_xH_{2x}

YIELD - percentage of fuel burned at time "zero"

The fixed point variable, MA, is the number of experimental runs with combinations of LH_2, RP-1, LO_2 and LF_2.

The Fortran IV program follows with an example of the output data for one of the nine data points using $LH_2/RP\text{-}1/LO_2/LF_2$ and entrained air.

Input Information

Many different quantities could have been chosen for the input information based upon which the desired fireball composition and atmospheric chemistry could be calculated.

For this investigation the

Volume-time history

Pressure-time history

Temperature-time history

were taken as the principal input information.

The reason for this choice was that another phase of this over-all program deals with the theoretical determination of these functions and most of all that it is possible to measure the above quantities and thus verify any theoretical results by actual field experimentation. This latter fact seems to be of extreme importance if theories are developed since without experimental verification they are of little use and certainly not much credence can be given to them.

Other factors such as fuel burning rates, etc. were selected by others (9,10) but the investigators of this project do not see how such quantities could be verified experimentally and therefore would remain assumptions throughout the work.

As mentioned above much work is being done on the determination of the volume-time, pressure-time, and temperature-time histories of the explosion phenomena from a theoretical point of view. Rather than wait for the results from this separate investigation and because of contract commitments it was decided to present the methods of obtaining the fireball and combustion cloud composition from such input data as mentioned above and for the present combine both theory and experimental information to obtain the most plausible functions at this time.

A brief description of how the volume-time, pressure-time, and temperature-time functions have been determined for this report follows.

Volume - Time History of Fireball and Combustion Products Cloud from Liquid Propellant Explosions

The volume of combustion products produced by liquid propellant explosions transgresses a number of stages with time, changing in shape from one typical configuration into another. These stages can be observed in the high speed film records of such explosions and can be, in part at least, analyzed mathematically or theoretically. These major stages are:

1. Hemisphere
2. Truncated Sphere
3. Sphere
4. Pinched Sphere
5. Toroid

The above 5 stages are distinct and can be observed in at least the larger explosions.

Stage 1 : Hemisphere

This stage is the earliest one which can be observed and is of relatively short duration. It involves a very rapid growth of the combustion products both along the ground and up into the atmosphere so that the shape can best be approximated by a hemisphere. The size of this initial hemisphere depends upon the yield of the liquid propellant explosion, the very rapid combination of the fuel and oxidizer so as to form detonation and shock waves. The larger the yield the larger the initial hemispherical fireball.

Stage 2 : Truncated Sphere

Following the very rapid formation of the hemispherical fireball from liquid propellant explosions the hot combustion products begin to rise. This upward motion and the convection currents due to the bouyant forces undercut the rising mass thus forming a truncated sphere, in contact with the ground at the flat base.

As the center of the mass rises the fireball changes more and more from the original hemisphere into a sphere, the shape which is attained when the combustion products become essentially tangent to the ground.

This stage in the development is referred to as "Lift Off", at which most of the fuel seems to have been consumed (9,10).

Stage 3 : Sphere

Having attained essentially a spherical configuration at "Lift Off" the combustion products continue to rise as a rather turbulent, well mixing sphere which however gradually changes shape from the almost perfect sphere into the first slightly pinched and then rather pronounced pinched sphere.

Stage 4 : Pinched Sphere

The change from the spherical configuration to the pinched sphere is rather gradual and then as the indentations become larger and larger, the appearance of the sphere is lost. A cross-section by a vertical plane through the center would give the appearance of a "Bar Bell."

As this process continues the indentations will eventually touch, forming a toroid.

Stage 5 : Toroid

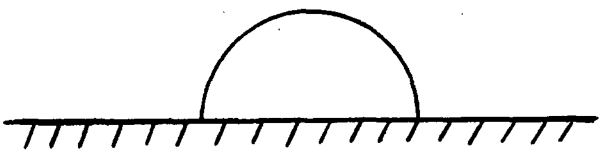
From the time the toroid is formed the initial contact point of the indentation becomes a hole with the general configuration of a ring or doughnut.

As this toroid grows in diameter the size of the hole increases but the volume now at this stage of development increases relatively slowly.

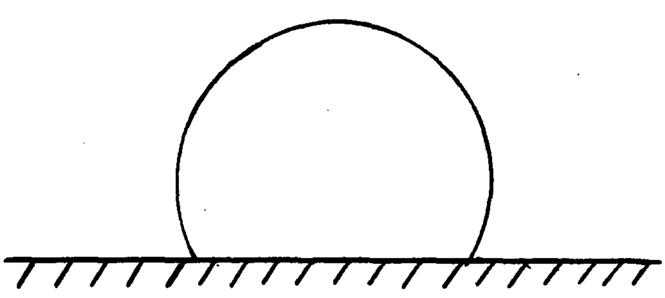
Finally this well defined configuration diffuses into the atmosphere losing its resemblance to any characteristic shape and being controlled to a great extent by the prevailing atmospheric conditions.

Each of these stages as described above and schematically shown in Fig. 1, takes a longer and larger part on the time scale. Stage 1 may occur in fractions of a second while the last stage will be a matter of minutes

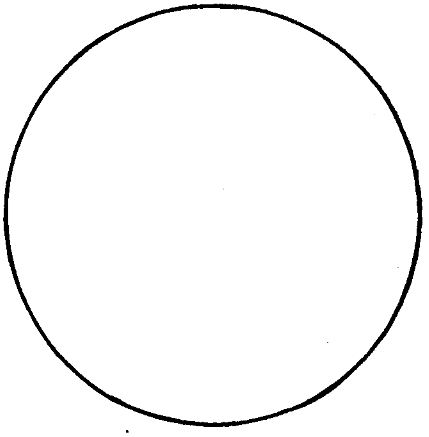
FIGURE 1-. TYPICAL DEVELOPMENTAL CONFIGURATION STAGES OF LIQUID PROPELLANT EXPLOSIONS



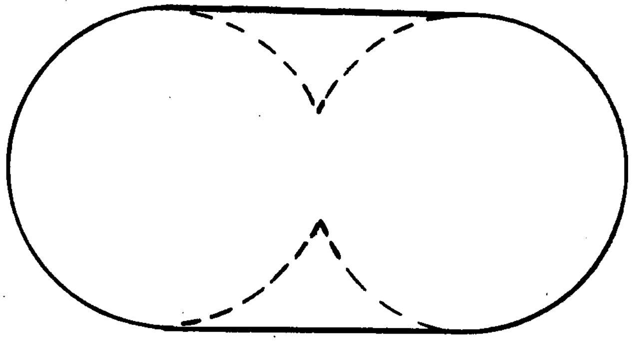
STAGE 1-. HEMISPHERE



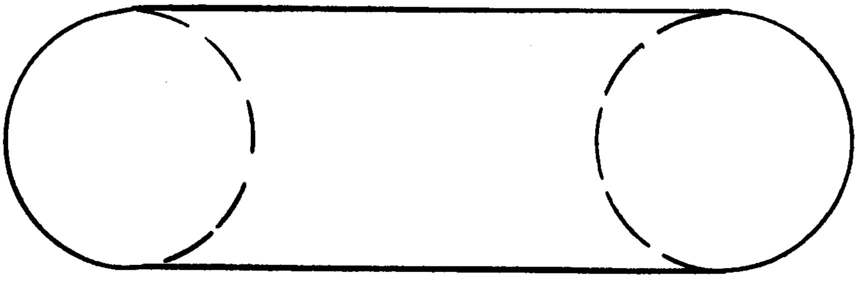
STAGE 2-. TRUNCATED SPHERE



STAGE 3-. SPHERE



STAGE 4-. PINCHED SPHERE



STAGE 5-. TOROID

Utilizing this 5 stage concept for the purpose of analysis a volume versus time curve can be obtained, either theoretically by the use of restricting assumptions or by the actual analysis of high speed film records of liquid propellant explosions.

The variation is greatest in stage 1 which is controlled by the yield while the statistical differences are rather small (but somewhat dependent upon atmospheric conditions) as long as the same quantities of propellants are involved and it is assumed that essentially all the propellants take part in the formation of the fireball and cloud (9,10).

Fig. 2 shows the volume versus time curve for the S-IV Pyro experiment. The yield as reported was about 4 1/2 % which is in agreement with the predictions of reference (1).

Similar volume versus time curves have been developed for the various fuel oxidizer combinations considered and reported upon here.

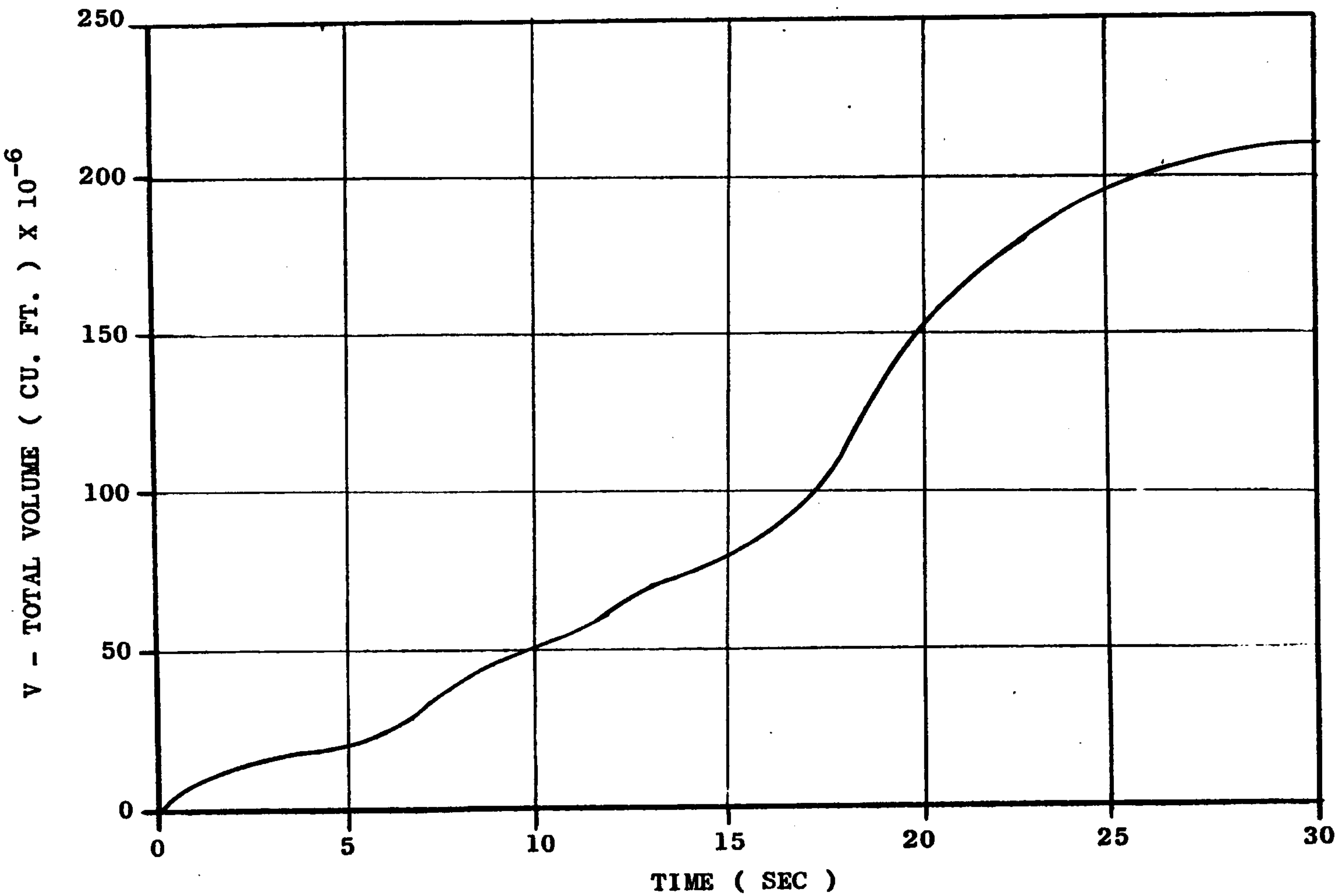


FIGURE 2-. TYPICAL VOLUME-TIME FUNCTION FOR LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

Pressure - Time History of Fireball and Combustion Products Cloud from Liquid Propellant Explosions

The pressure - time history as presented here and as used as input data for the determination of the composition of both the fireball and the combustion products cloud was determined partially from preliminary theoretical considerations (8) and partially from the analysis of field data obtained by the liquid propellant explosion program of project PYRO (12).

The theoretical analysis was necessary for the early time processes since no experimental data is available and the results were then checked and agreed with experimental results in the later stages.

In general it might be said that the pressure immediately after ignition rises very rapidly to very high values inside the missile due to the confinement of the propellants and the tanks, reaching a maximum some where as the reaction front progresses toward the boundary of the missile configuration. After this maximum is reached the pressure falls very rapidly to almost atmospheric conditions.

From the time of "Lift-Off" of the fireball which occurs at essentially atmospheric pressure (13) the pressure drops very slowly due to the rise of the explosion products and the effect on atmospheric pressure due to altitude.

The pressure - time history presented here for approximately 100,000 lbs of propellants was used for all the propellants reported upon here.

Analysis of the sparse experimental information of liquid propellant explosion experiments seems to support this general pressure - time history. The yield produced by the explosion will change the early values of the pressure. Again for the analysis here a yield of 4 1/2 % was taken based upon the most likely value as given in reference (5).

The actual curve used here is presented in Fig. 3. If better information is to be used an experimental program could be instituted to actually measure these pressures, an important reason for this choice of input information is because it allows theoretical determination and experimental verification.

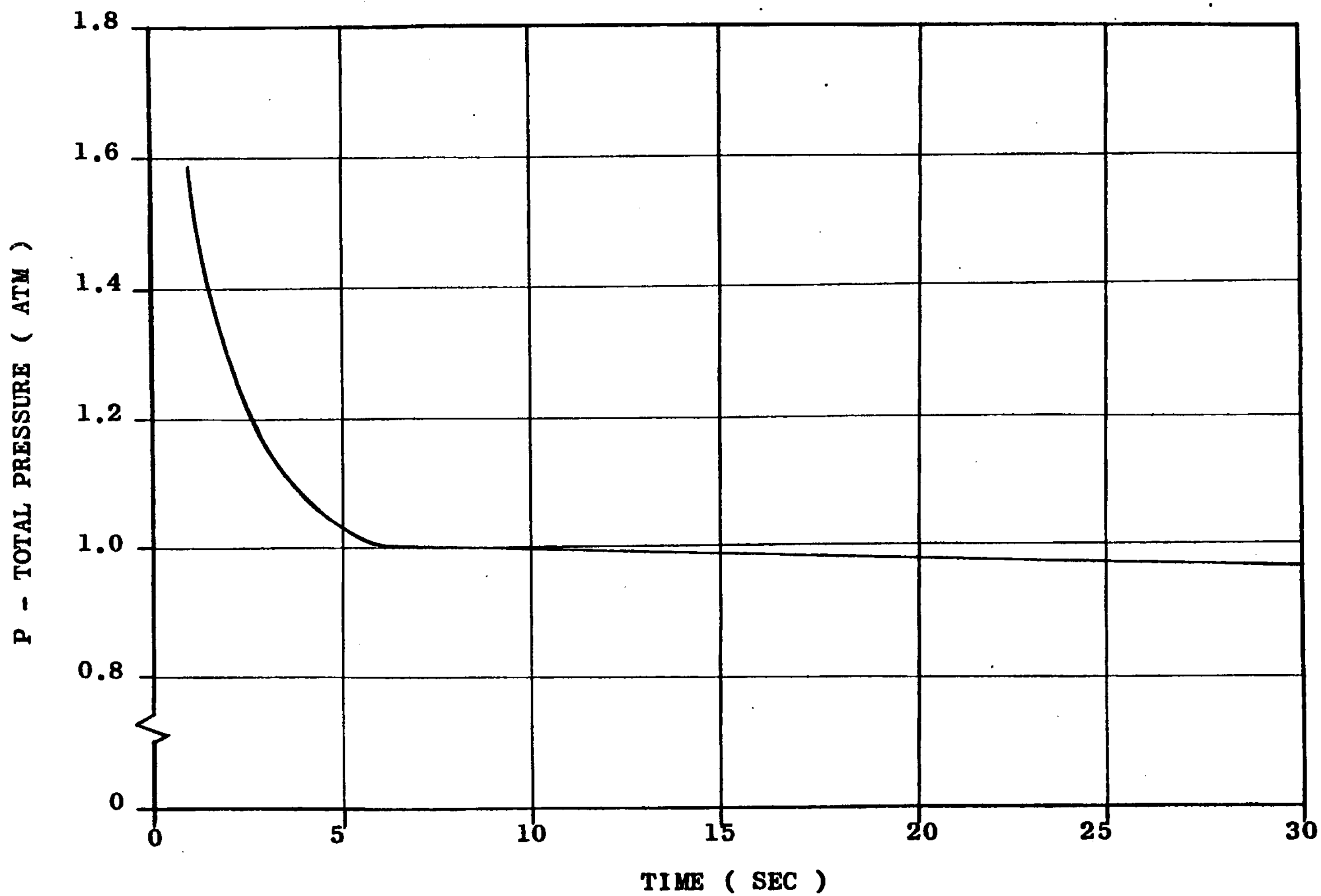


FIGURE 3-. TYPICAL PRESSURE-TIME FUNCTION FOR LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

Temperature - Time History of Fireball and Combustion Products Cloud from Liquid Propellant Explosions

The third and last principal input information needed for the determination of the composition of the fireball and combustion products cloud including air entrainment and atmospheric interaction is the temperature - time relationship.

Again theoretical considerations and the available rough experimental observations of fireball temperatures and variations with time indicate that the initial temperature is close to the maximum obtainable by the particular propellants involved. Then, at low yields at least, since only a small part of the propellants take part in the initial stages of the fireball formation the reaction of the remaining fuel and oxidizer, both in the propellants as well as the atmosphere, make the temperature drop with temperature in an almost linear manner. This is observed in theoretical work (9,10) and seems to be closely approximated by the available experimental information (12).

This linear decrease of the temperature with time continues until the incandescence of the fireball ends often referred to as the "duration" which can be approximated as shown in (13).

For the purpose of analysis here it was assumed that the actual variation can be closely approximated by further linear decreases changing the slope to a value 1/2 the previous one for each subsequent "duration" time interval.

By this method a curve representing the temperature-time history of the liquid propellant explosion is obtained which from both theoretical and the available sparse experimental observations seems to approximate the actual conditions. This again is taken here for low yield (4 1/2 % in this case) liquid propellant explosions.

Again it is believed that an experimental program can be designed, if desired, to obtain this temperature - time history for various cases and verify or modify the presently used information, which is presented in Fig. 4 and again was used for all the fuel - oxidizer combinations analyzed and reported upon here.

It should be mentioned again that the volume-time, pressure-time, and temperature-time histories were selected as the principal input data because it is felt by these investigators that this information which can be generated with appropriate assumptions theoretically, can be verified experimentally. In addition these volume-time, pressure-time, and temperature-time histories are of great interest to other investigators for various reasons. A number of groups are presently engaged in trying to measure pressures and

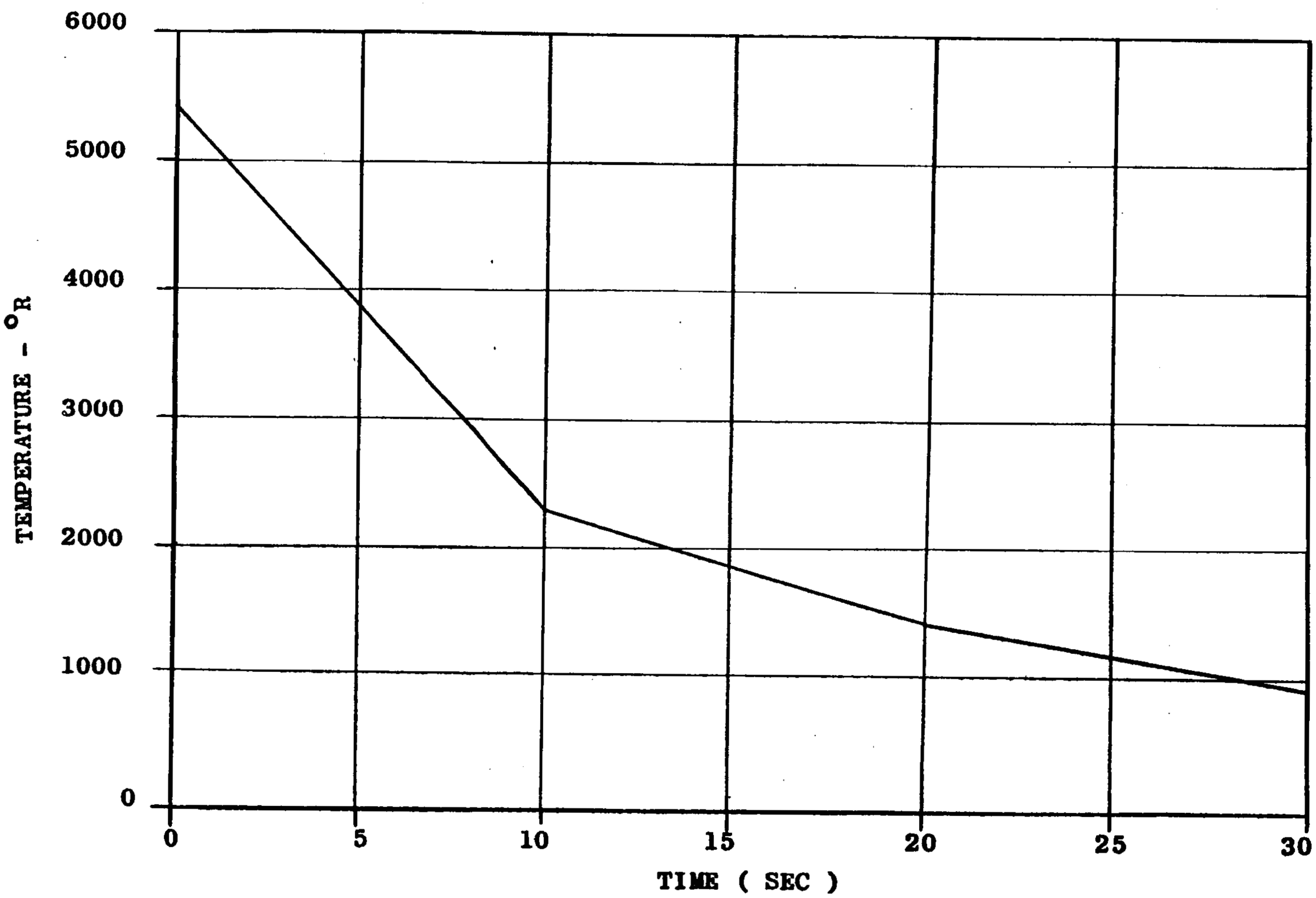


FIGURE 4-. TYPICAL TEMPERATURE-TIME FUNCTION FOR LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

temperatures within fireballs and of combustion products clouds produced by liquid propellant explosions.

It should also again be emphasized that in this investigation homogeneity of the fireball as well as of the combustion products cloud was assumed. These assumptions seem to be reasonably well satisfied because of the tremendous turbulence observed within the fireball which tends to produce thorough mixing within a relatively short time.

In addition to the principal input information, the volume-time, pressure-time, and temperature-time functions it is necessary to know

4. The Type of Propellants
5. Propellant Composition
6. Propellant Quantities
7. Yield

4,5, and 6 are easily obtainable as original data, while 7 is selected to obtain the results for this particular value of yield, a value which may again be dictated by theoretical considerations.

Type of Propellants

The type of propellants selected for this presentation are combinations of fuel and oxidizers which are presently used in liquid propelled rocket systems or combinations which may become important in the future development of these rockets.

The method however used is perfectly general and any propellant type and combinations could be analyzed in the same manner.

The types selected for this presentation are:

LH_2/LO_2

RP-1/LO_2

LH_2/LF_2

RP-1/LF_2

LH_2/RP-1/LO_2

LH_2/LO_2	+	1% F
	+	5% F
	+	10% F
RP-1/LO_2	+	1% F
	+	5% F
		10% F
LH_2/RP-1/LO_2	+	1% F
	+	5% F
	+	10% F

Propellant Composition

The propellant type was outlined above with the composition of fuel to oxidizer chosen as follows:

LH_2/LO_2	1 : 5	by weight
$RP-1/LO_2$	1 : 2.25	by weight
LH_2/LF_2		
$RP-1/LF_2$		
$LH_2/RP-1/LO_2$	1 : 2.6 : 5.86	by weight

In the combinations with Fluorine traces the weight ratios of the main constituents were the same as given above.

The chemical composition of the RP-1 was taken as $C_{11.6}\ H_{23.2}$ which was obtained from reference (14).

Propellant Quantities

The propellant quantities were taken as 100,000 lbs in all cases. This allowed the standardization of the pressure-time and temperature-time histories for the present analysis, since it seems that the quantity of propellants used has the major effect on the time axis of pressure and temperature.

Yield

The yield, the energy release as a fraction of the theoretical maximum, for these calculations and analyses was taken as 4 1/2 % which from previous theoretical investigations (5) and from experimental observations (5,12) seems to come close to the statistically most probable value.

Again it might be mentioned that other values could be taken just as well without changing the method of analysis. The resulting compositions of the fireball and explosion products cloud would, however, be different.

With the input information as described above a number of cases were analyzed and many quantities calculated. Rather elaborate computer programs were developed for this purpose and the main program will be presented in the appendix.

The results which seem to be most pertinent to this investigation are presented in the following pages, mostly in graphical form.

Results Obtainable

Utilizing the data information as discussed above and the calculation and analyzing procedures outlined earlier many important quantities can be calculated.

Because of space limitations only the ones most pertinent to this investigation will be presented here. They are only a small fraction of all the quantities calculated but even though they form about 70 graphs many of them with a number of individual curves on them.

As mentioned earlier the same pressure-time, and temperature-time history was used for all the propellant combinations presented here, but individual volume-time histories for each type of propellant had to be calculated.

Then through a rather large iterative computer program such quantities as partial moles, partial pressures, partial volumes, partial weights, volume of air entrained, weight of air entrained, unburned fuel present, etc., were calculated.

Some of these quantities were then normalized and a few of them are presented here graphically as a function of time. They are

a. Fuel and oxidizer consumption, wgt. (Normalized)

b. Volume of entrained air (Normalized)

c. Partial pressures (Normalized)

d. Partial volumes (Normalized)

e. Partial weights (Normalized)

These results and the manner of presentation, it is believed, give a good picture of the composition and its time variation of the fireball and the combustion products cloud for 14 different propellant combinations.

It is believed that the graphs are self-explanatory and the characteristics of the different fuel-oxidizer combinations can easily be compared.

The Fluorine tracer quantities added seem to have a hypergolic effect upon the cryogenic propellants to render the prediction of the most probable ignition and delay times and thus yield more certain.

Presentation of Selected Results

LH_2 / LO_2

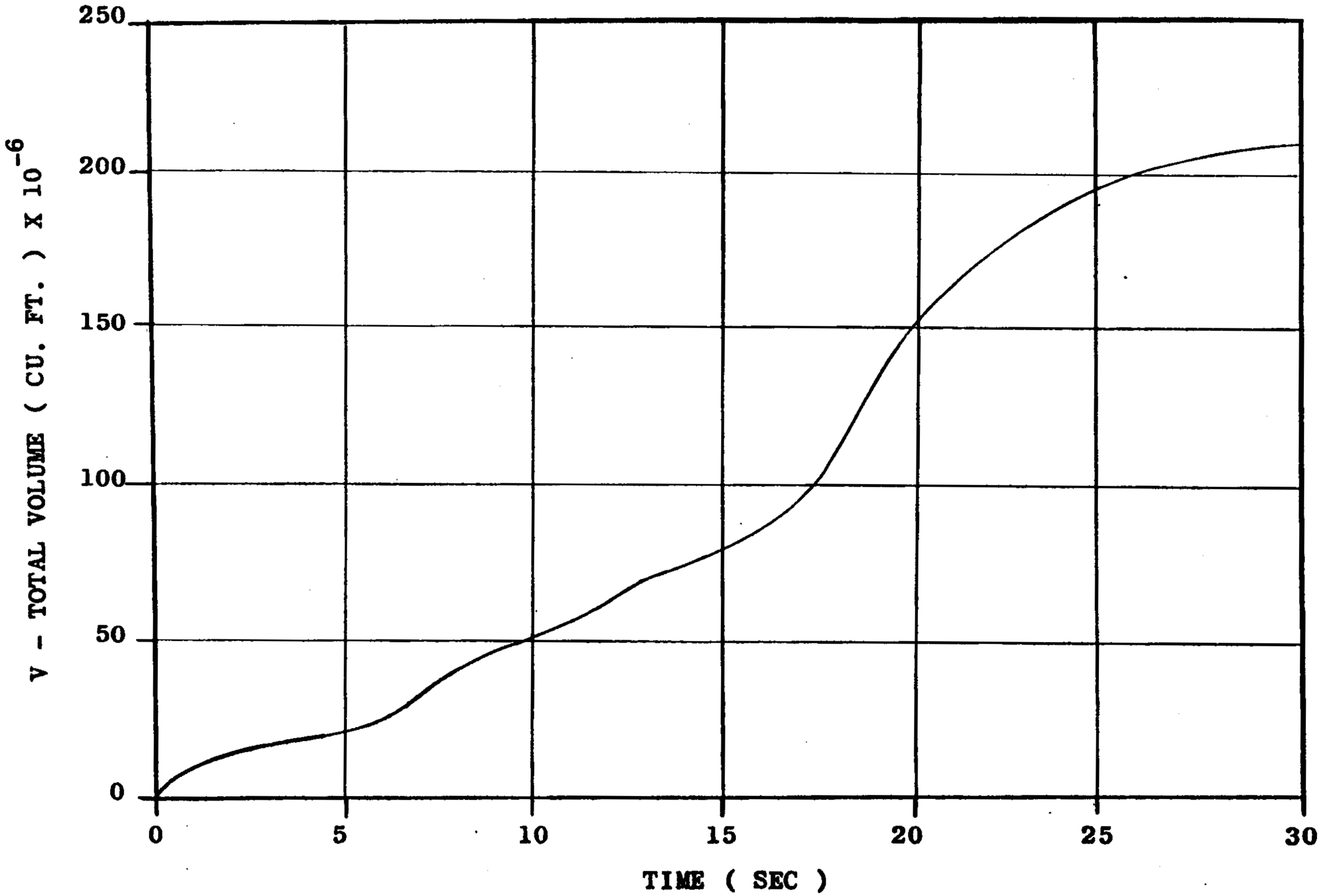


FIGURE 5 -. VOLUME-TIME FUNCTION FOR LH_2/ LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

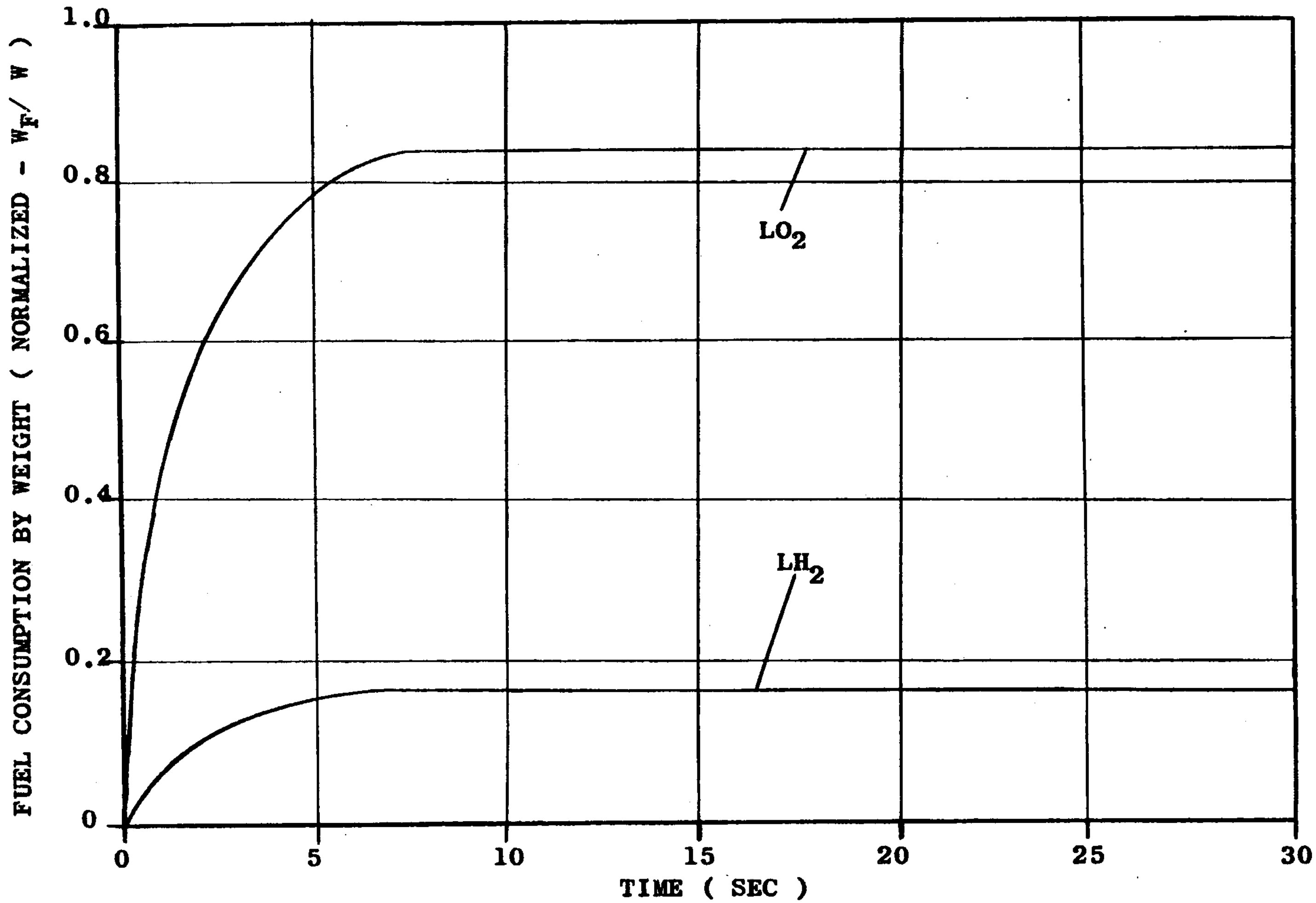


FIGURE 6-. FUEL CONSUMPTION FOR LH_2/ LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

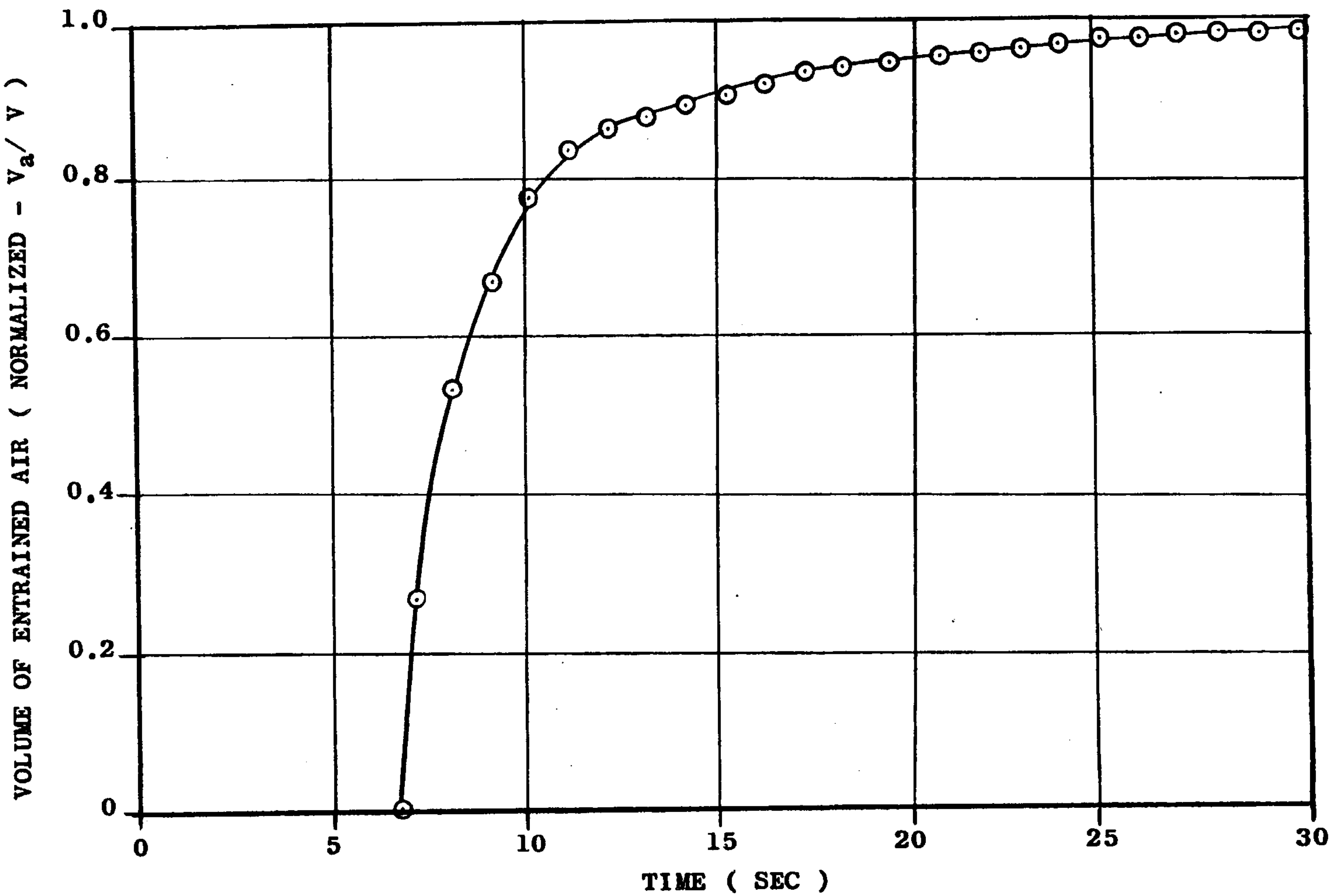


FIGURE 7-. VOLUME OF ENTRAINED AIR FOR LH_2/ LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

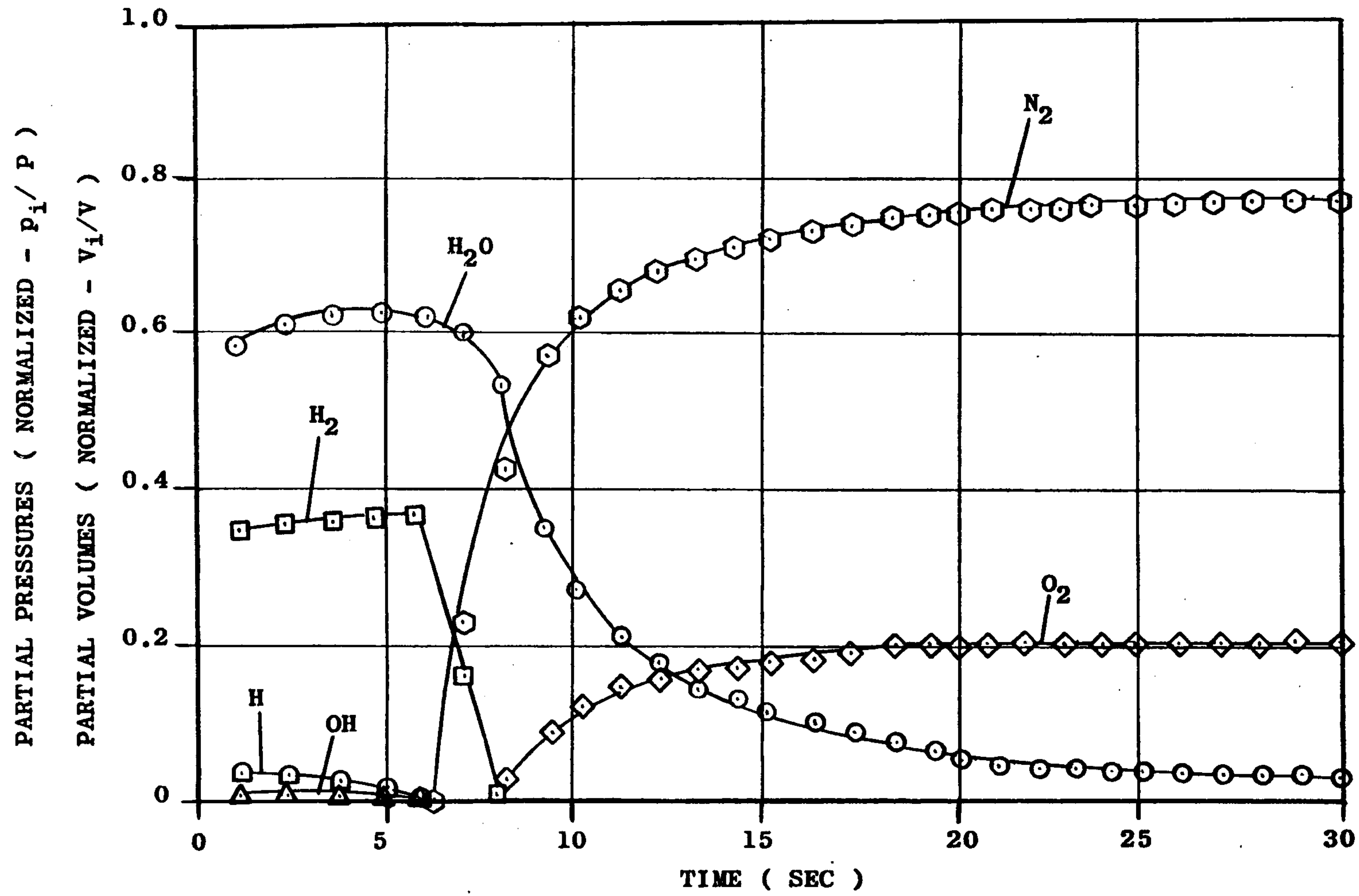


FIGURE 8-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/ LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

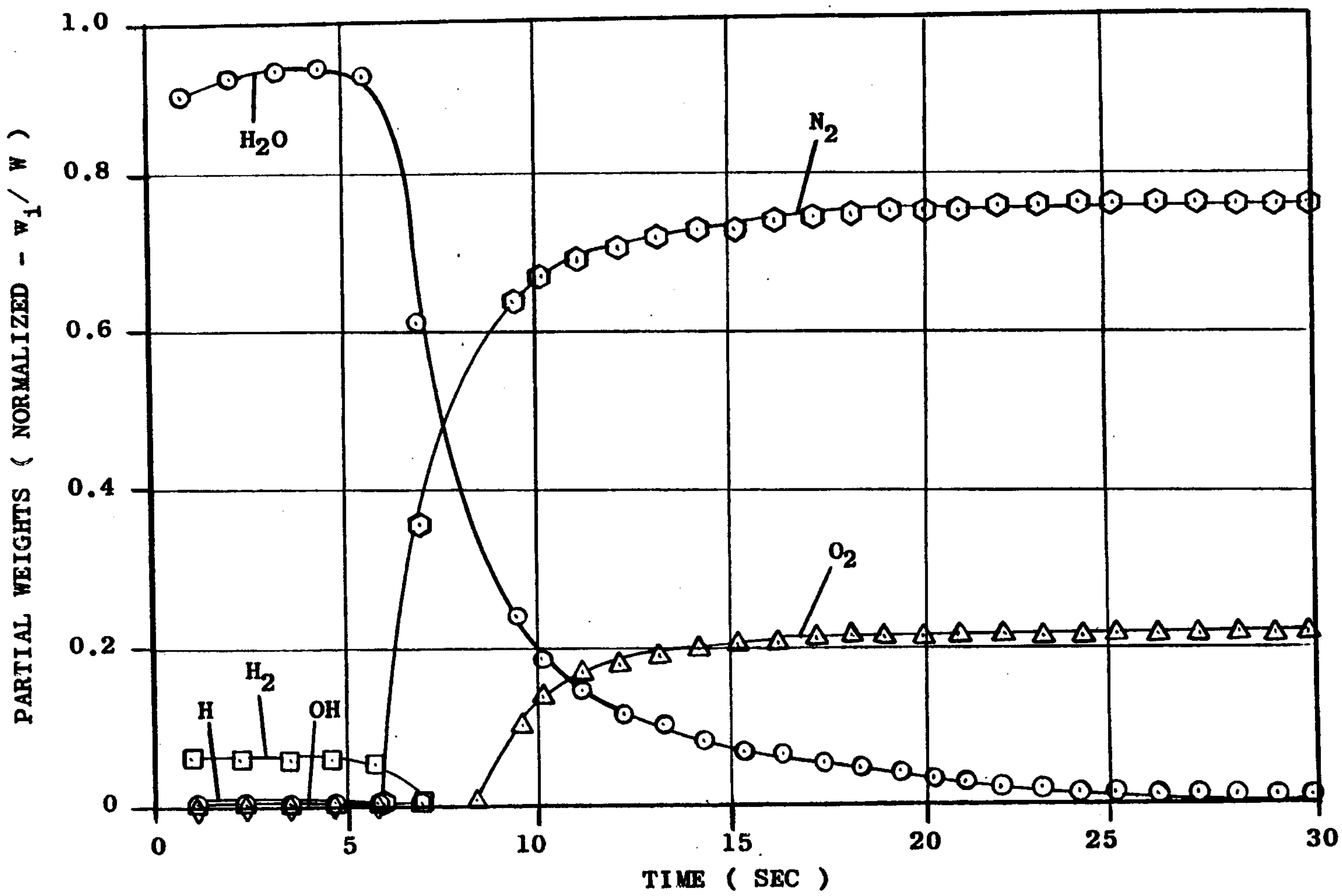


FIGURE 9-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/ LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

RP-1 / LO_2

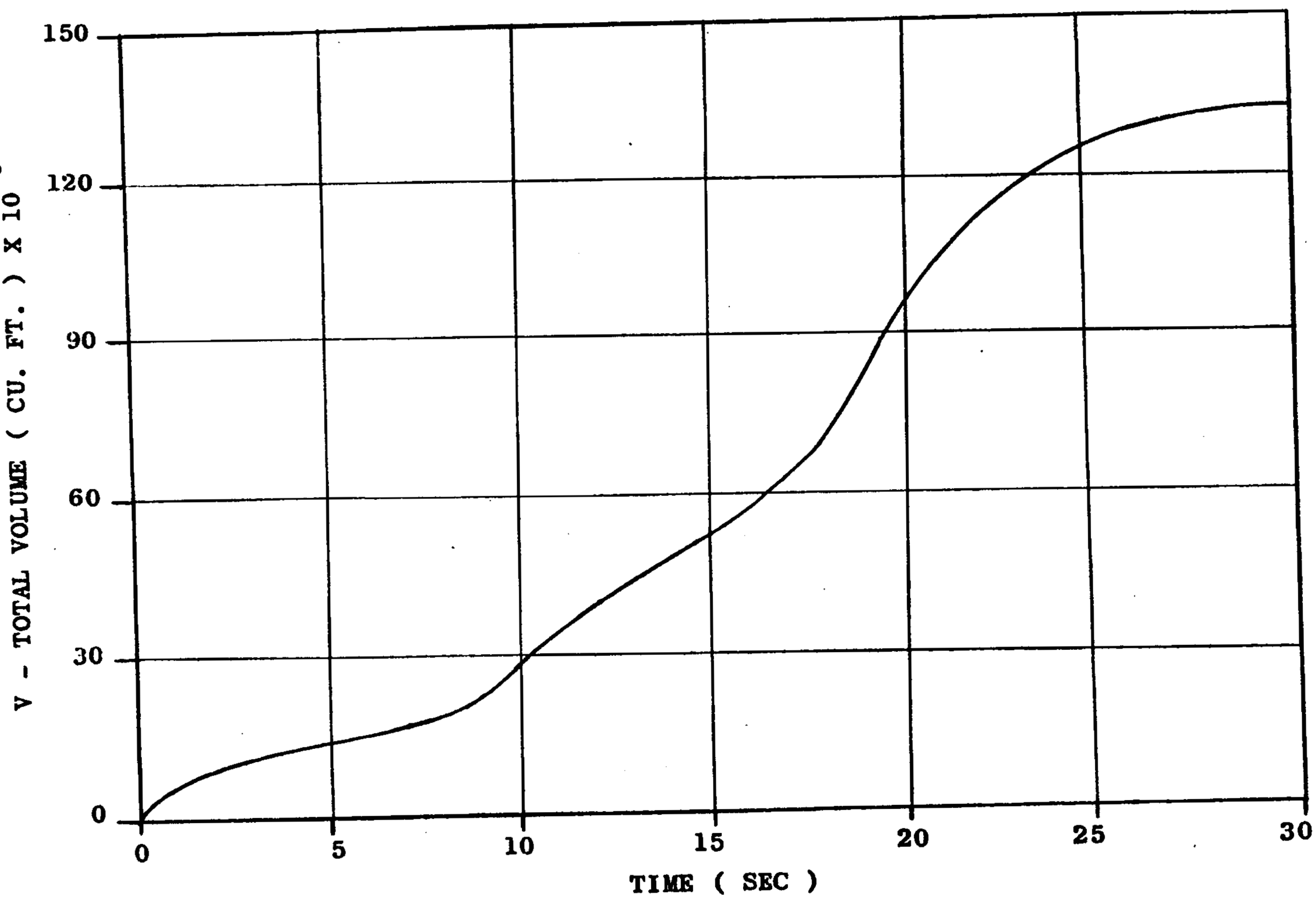


FIGURE 10-. VOLUME-TIME FUNCTION FOR RP-1/LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

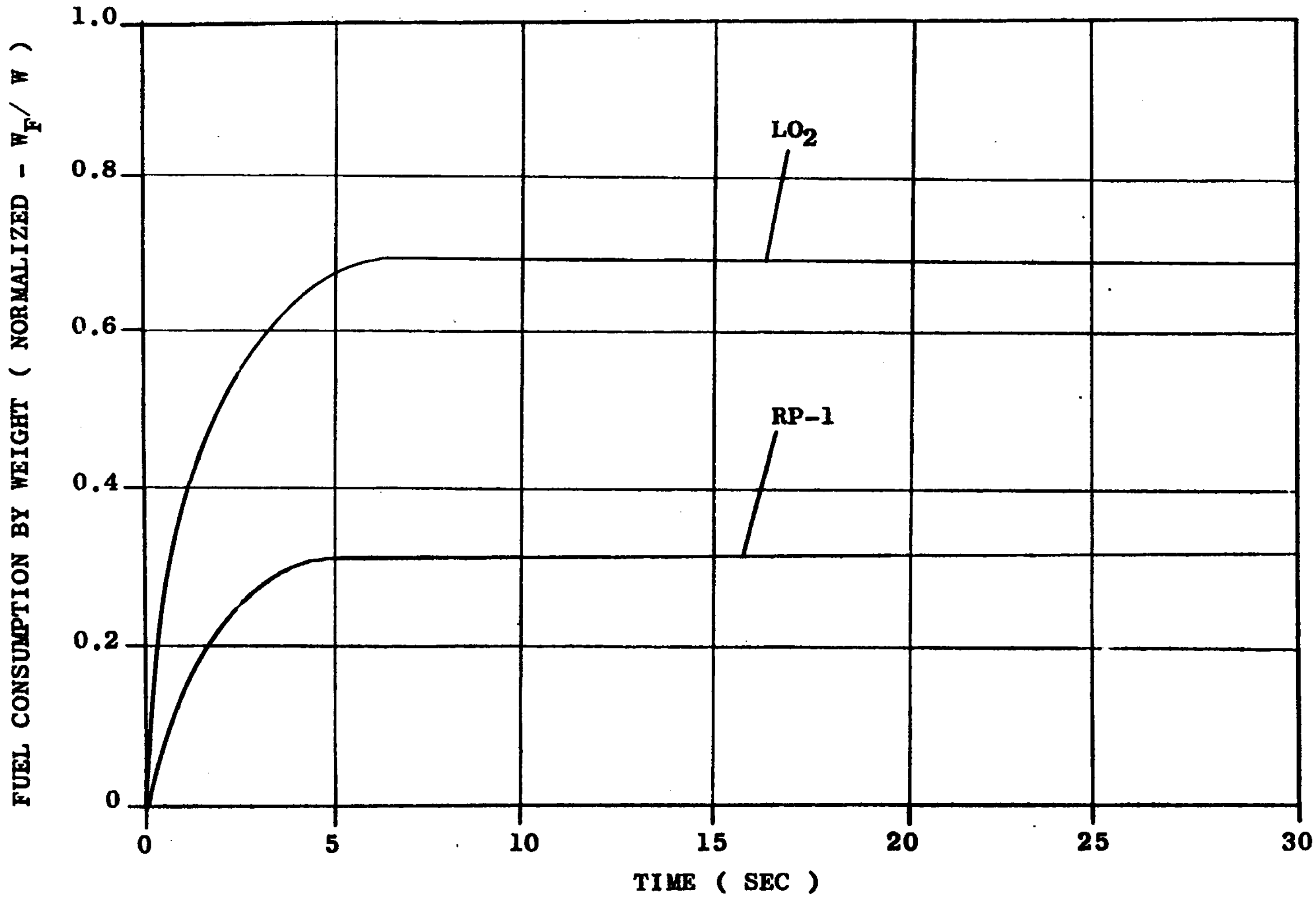


FIGURE 11-. FUEL CONSUMPTION FOR RP-1/LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

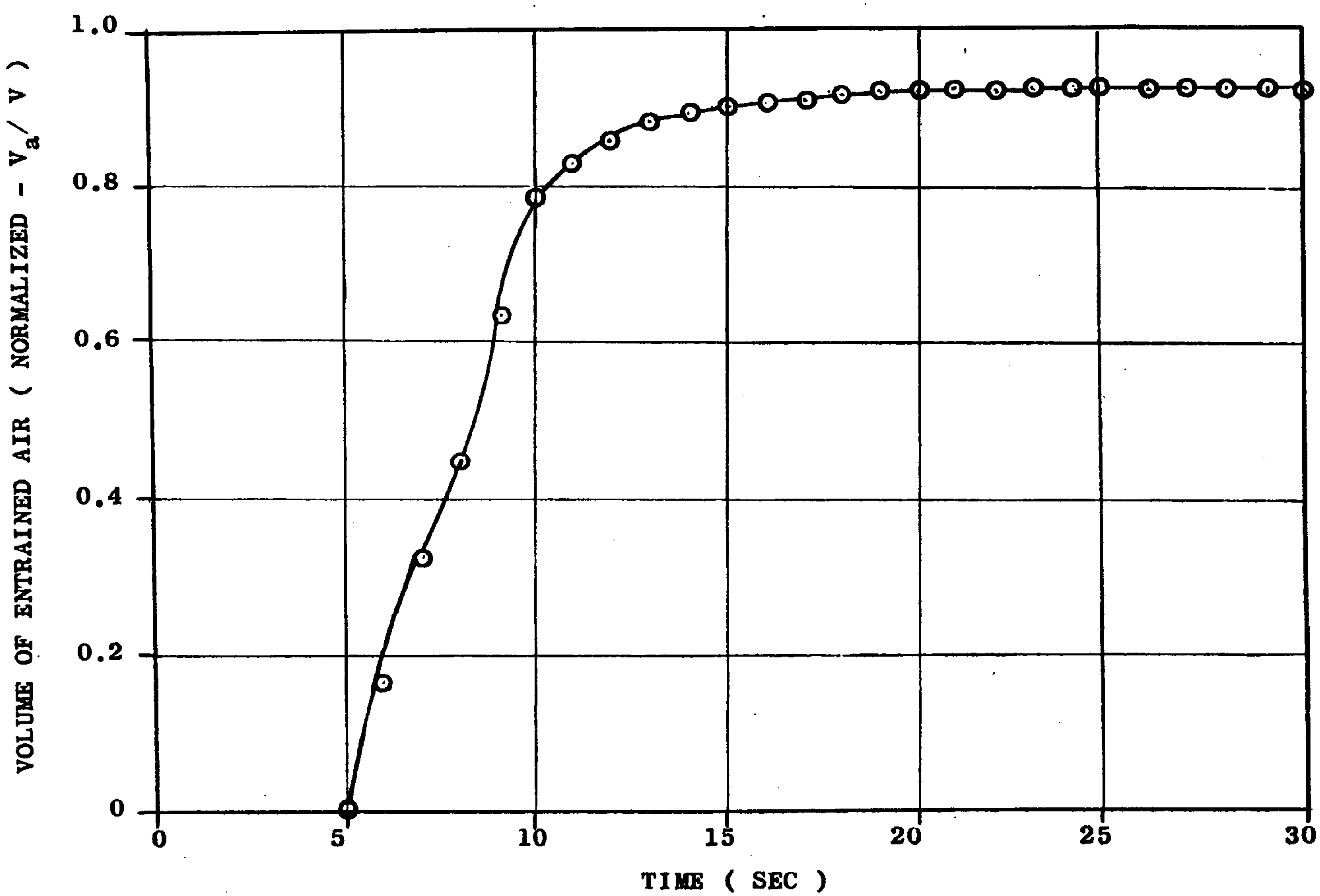


FIGURE 12-. VOLUME OF ENTRAINED AIR FOR RP-1/ LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

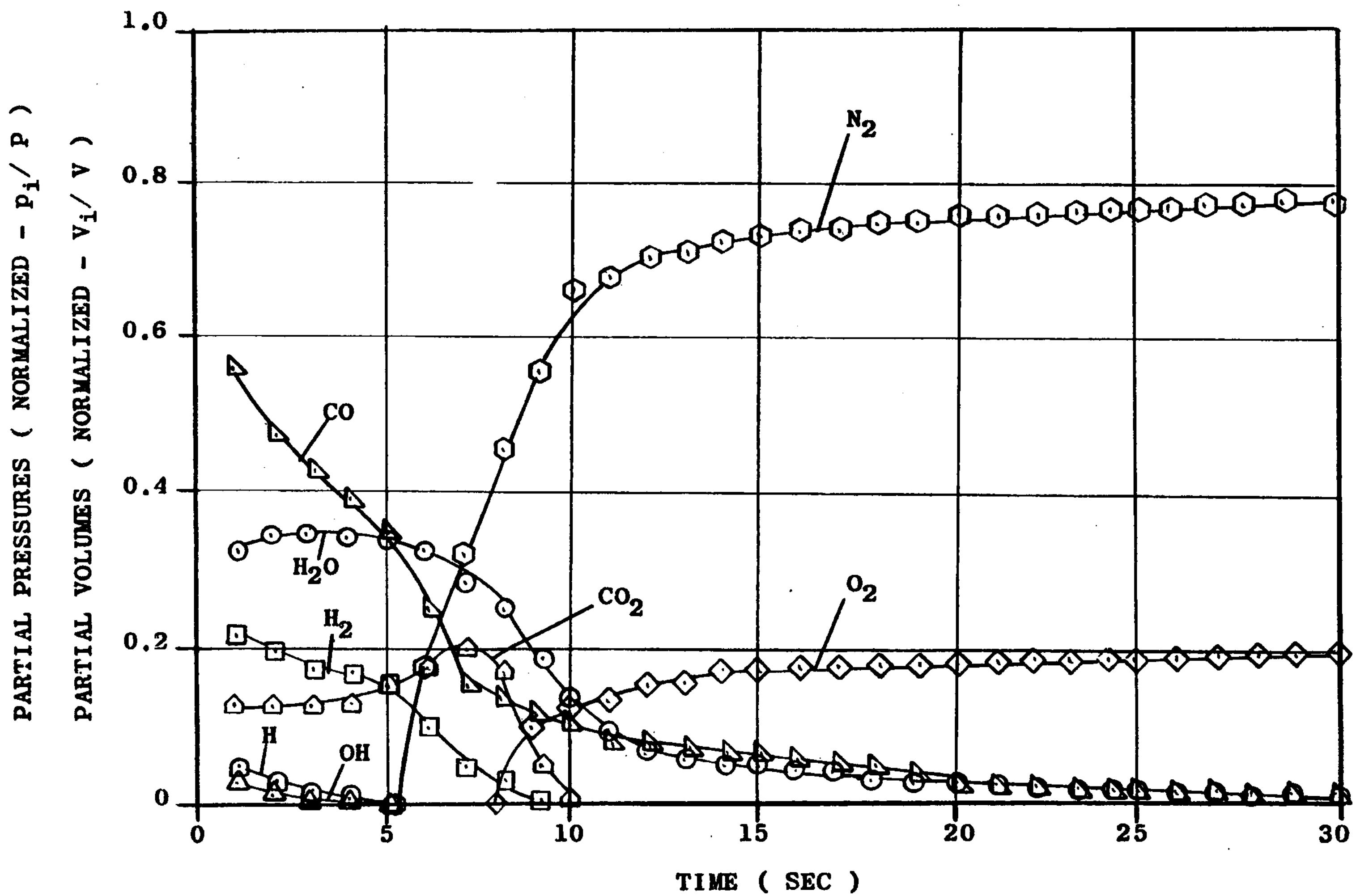


FIGURE 13-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR RP-1/ LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

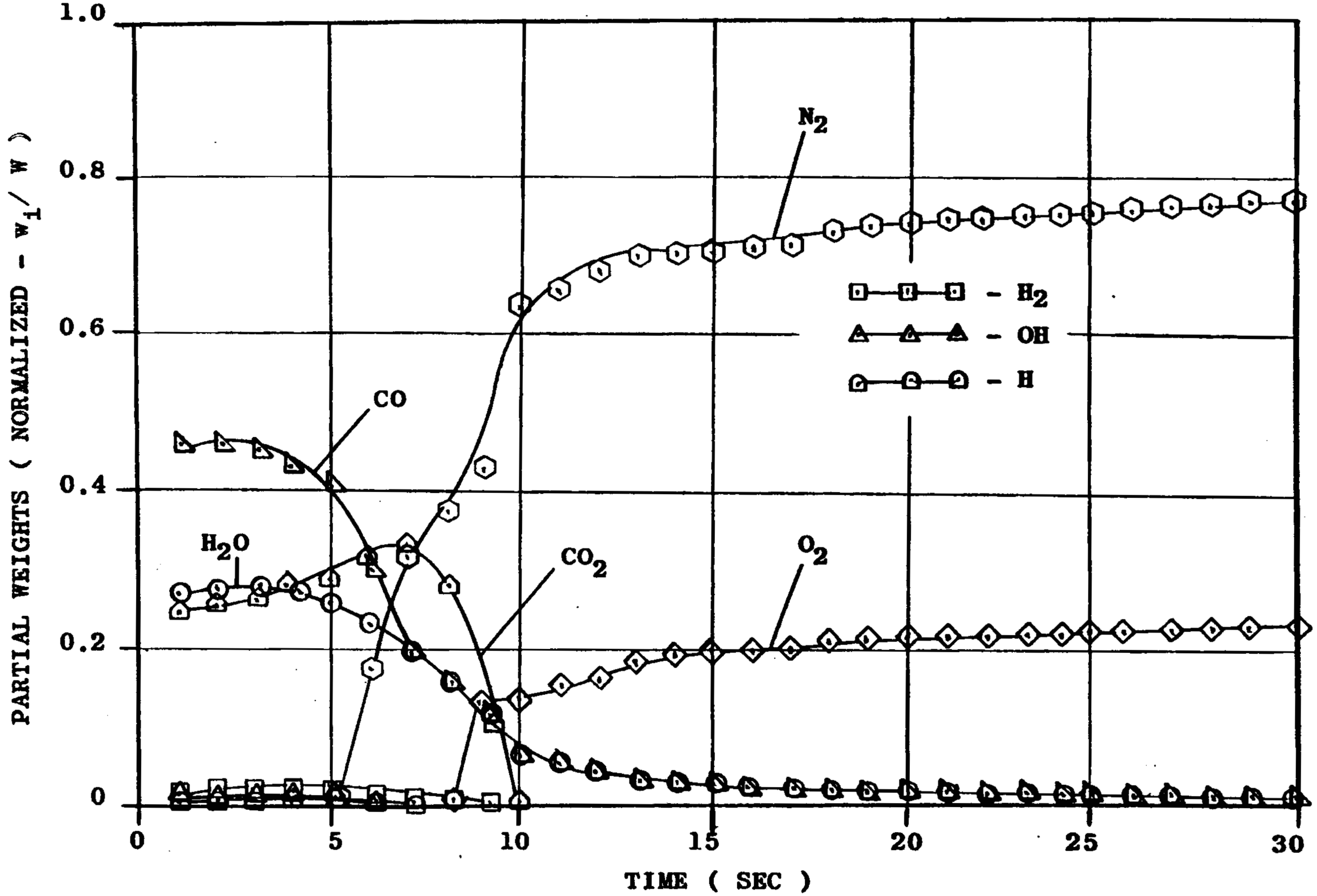


FIGURE 14-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM RP-1/ LO_2
LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

LH_2 / LF_2

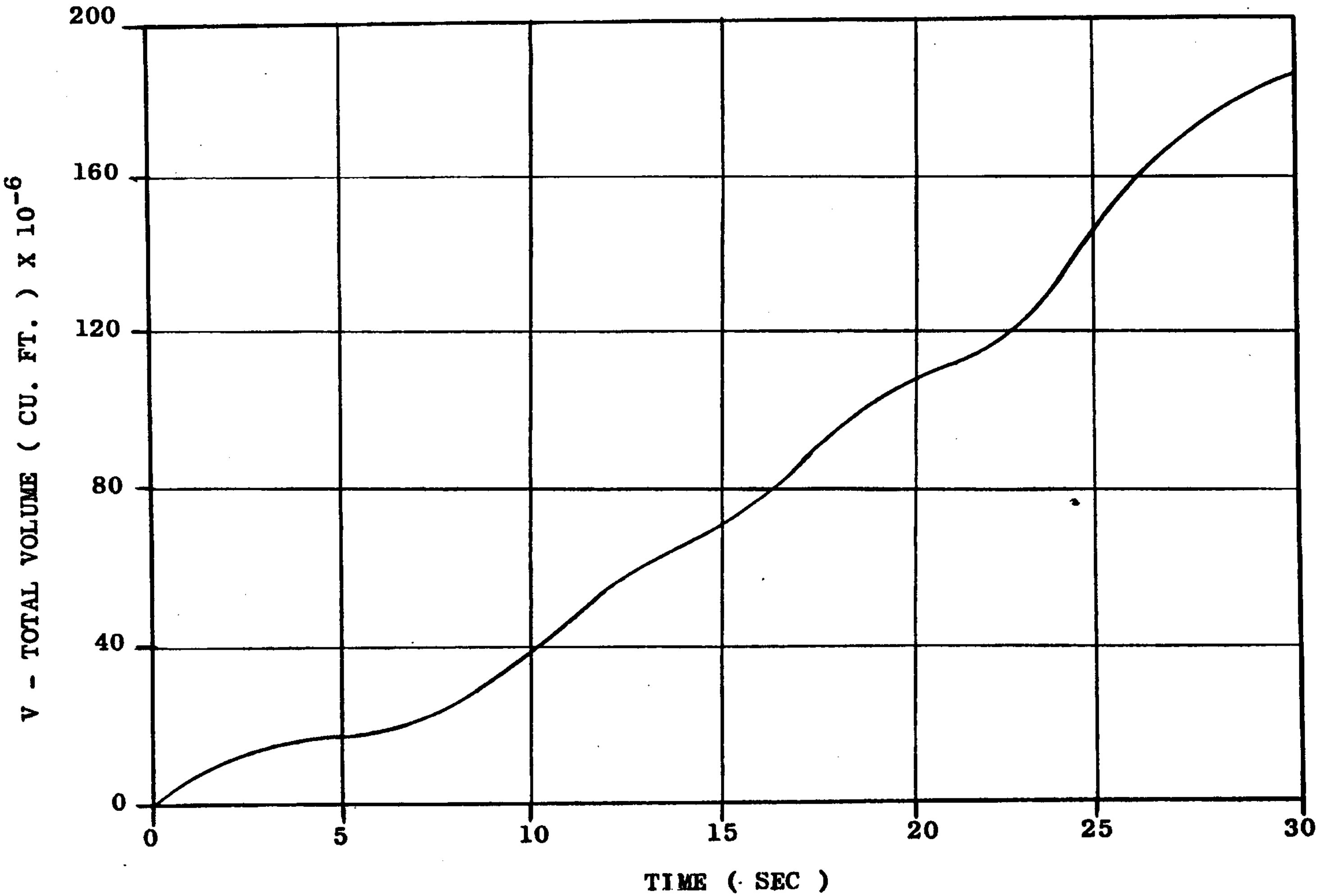


FIGURE 15-. VOLUME-TIME FUNCTION FOR LH_2/LF_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

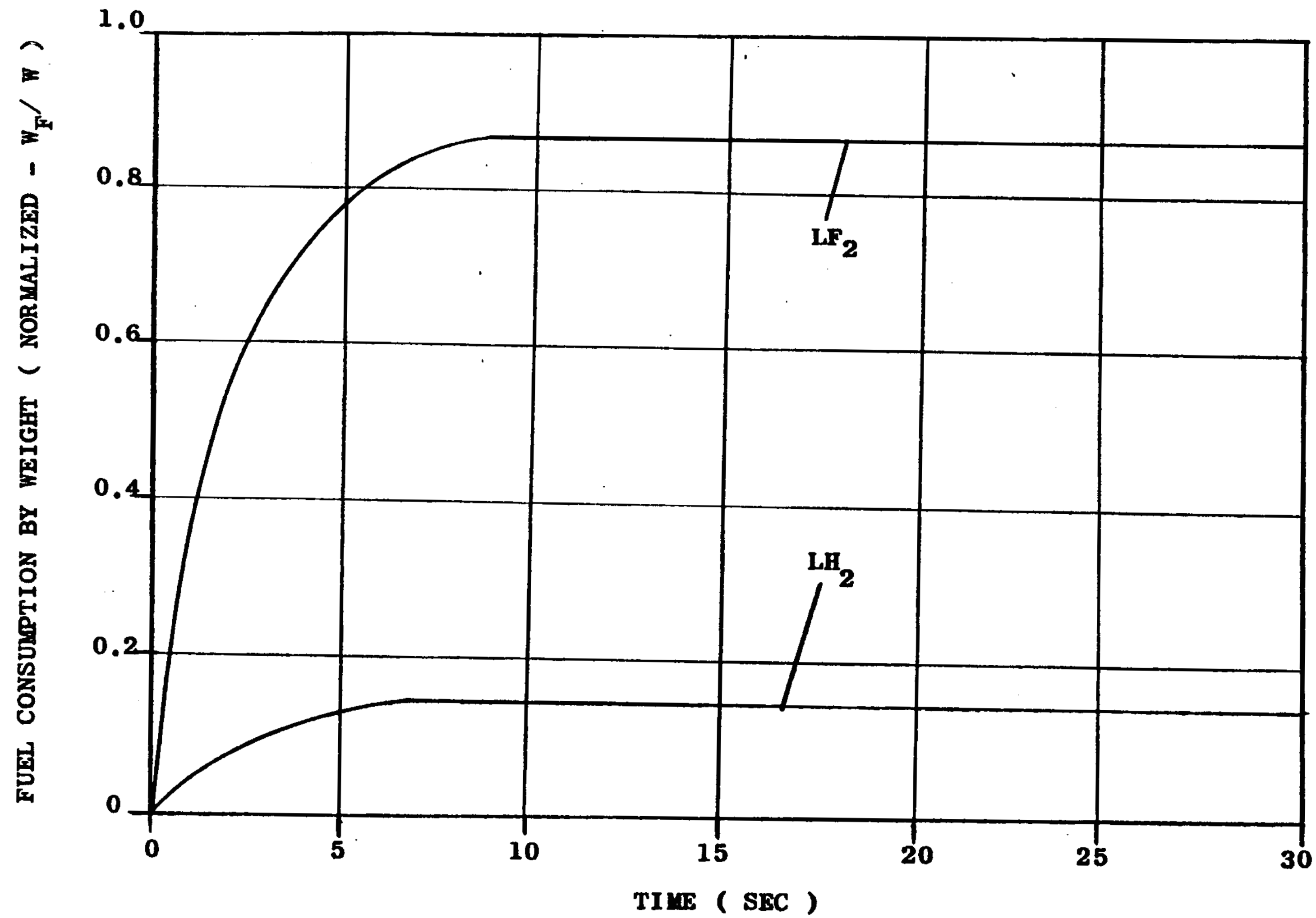


FIGURE 16-. FUEL CONSUMPTION FOR LH_2/LF_2 LIQUID PROPELLANT EXPLOSION

(YIELD = 4.5 PERCENT)

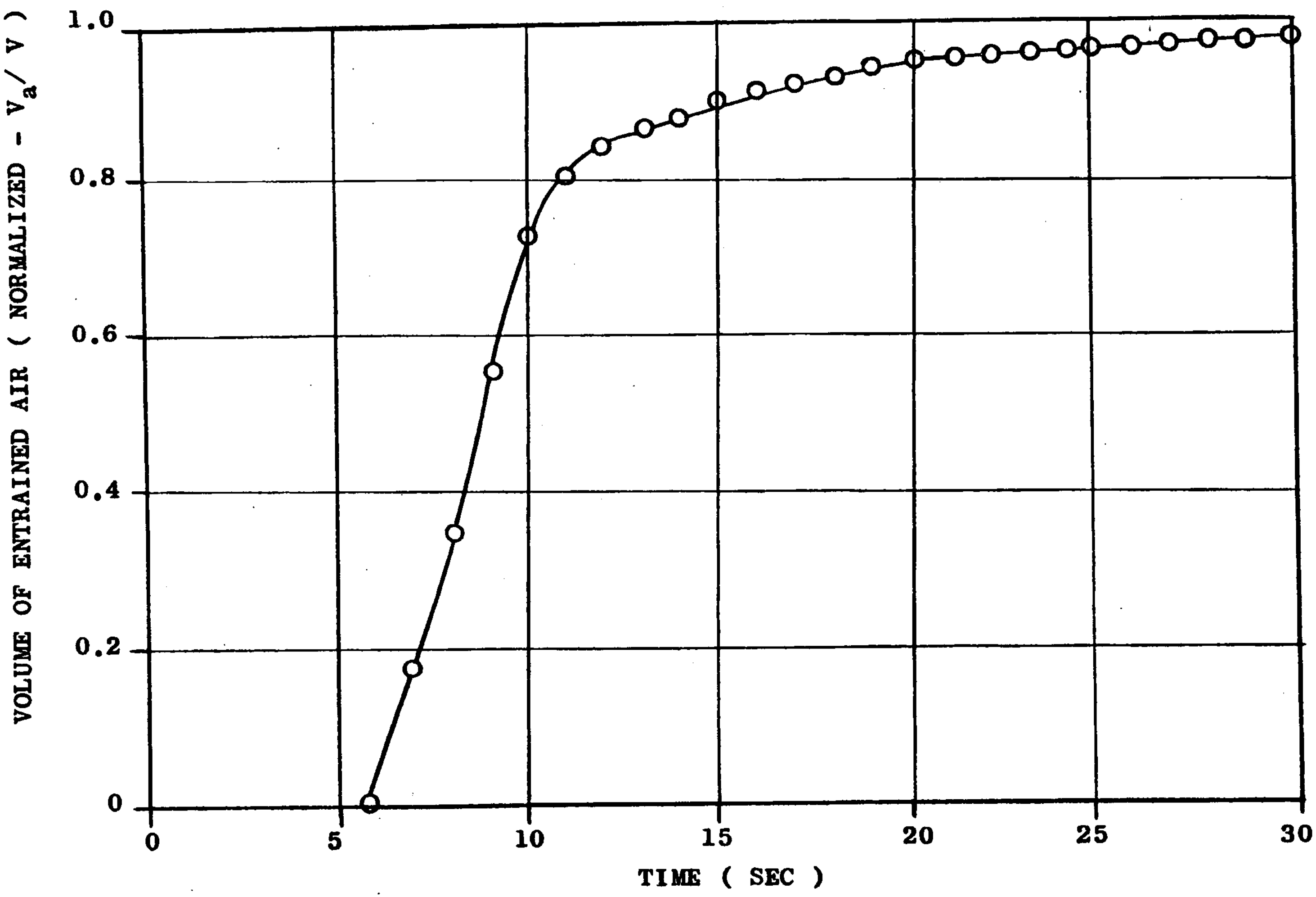


FIGURE 17-. VOLUME OF ENTRAINED AIR FOR LH_2/LF_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

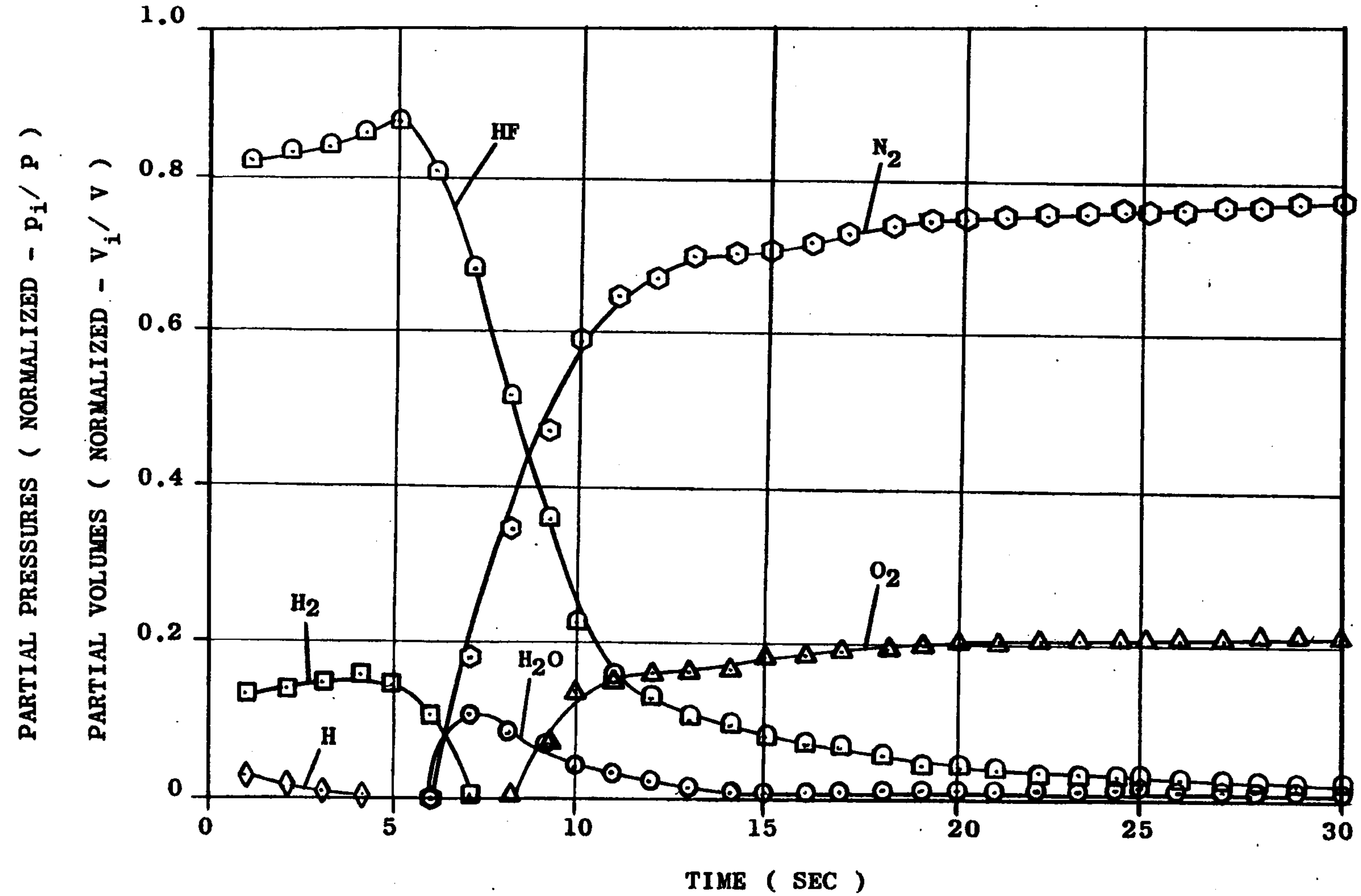


FIGURE 18-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/LF_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

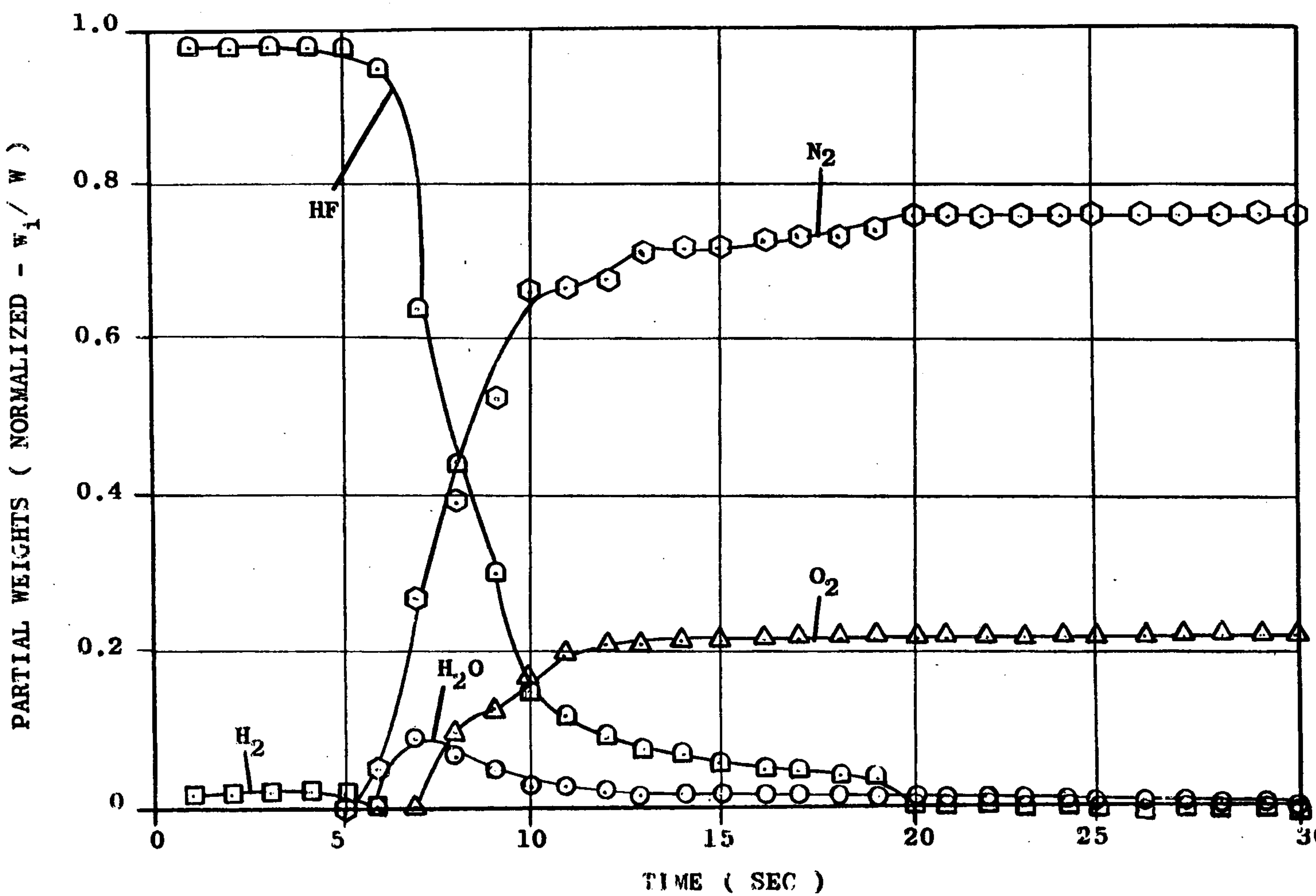


FIGURE 19-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/ LF_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

RP-1 / LF_2

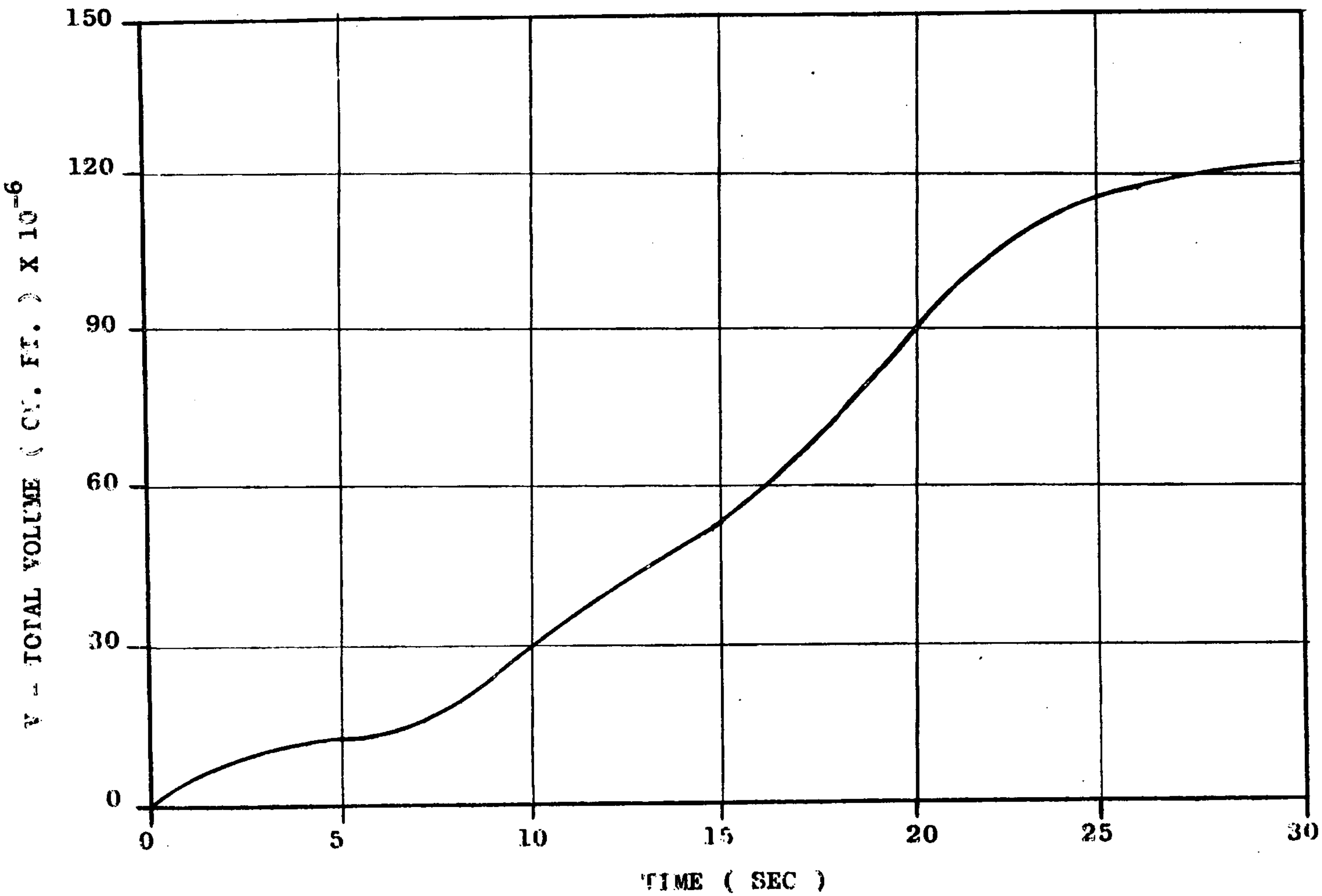


FIGURE 20-. VOLUME-TIME FUNCTION FOR RP-1/LF$_2$ LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

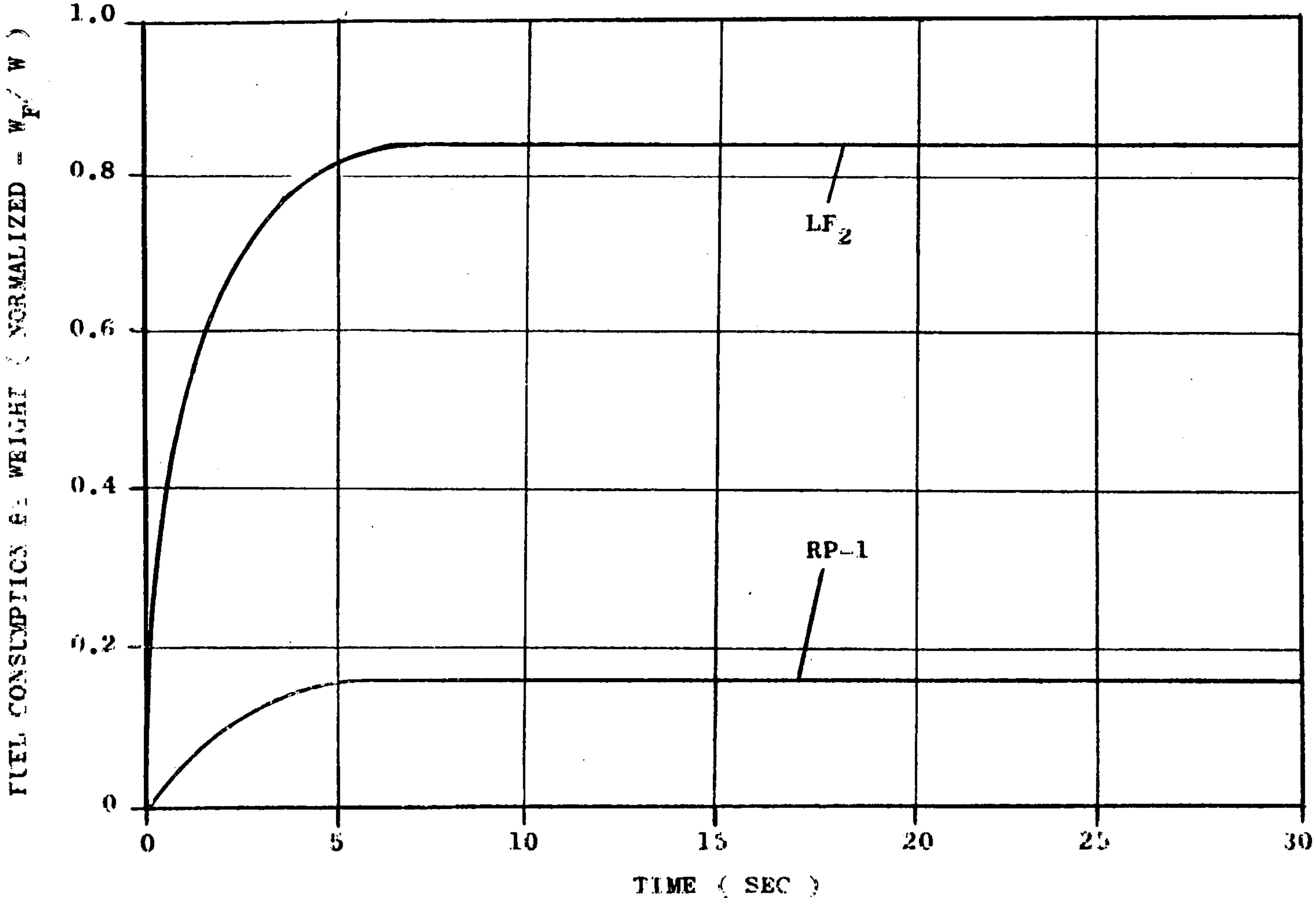


FIGURE 21-. FUEL CONSUMPTION FOR RP-1/LF_2 LIQUID PROPELLANT EXPLOSION

(YIELD = 4.5 PERCENT)

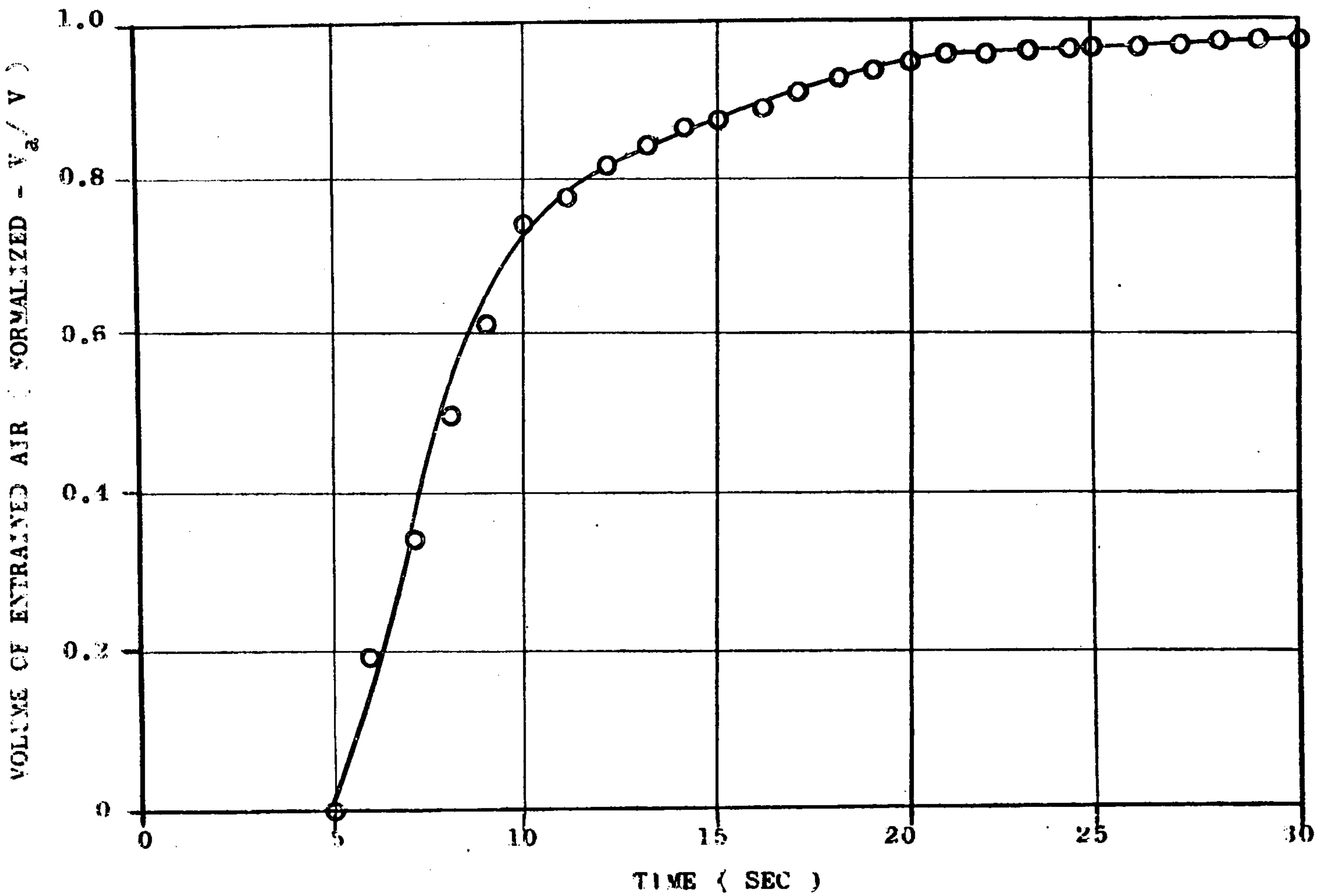


FIGURE 22-. VOLUME OF ENTRAINED AIR FOR RP-1/LF_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

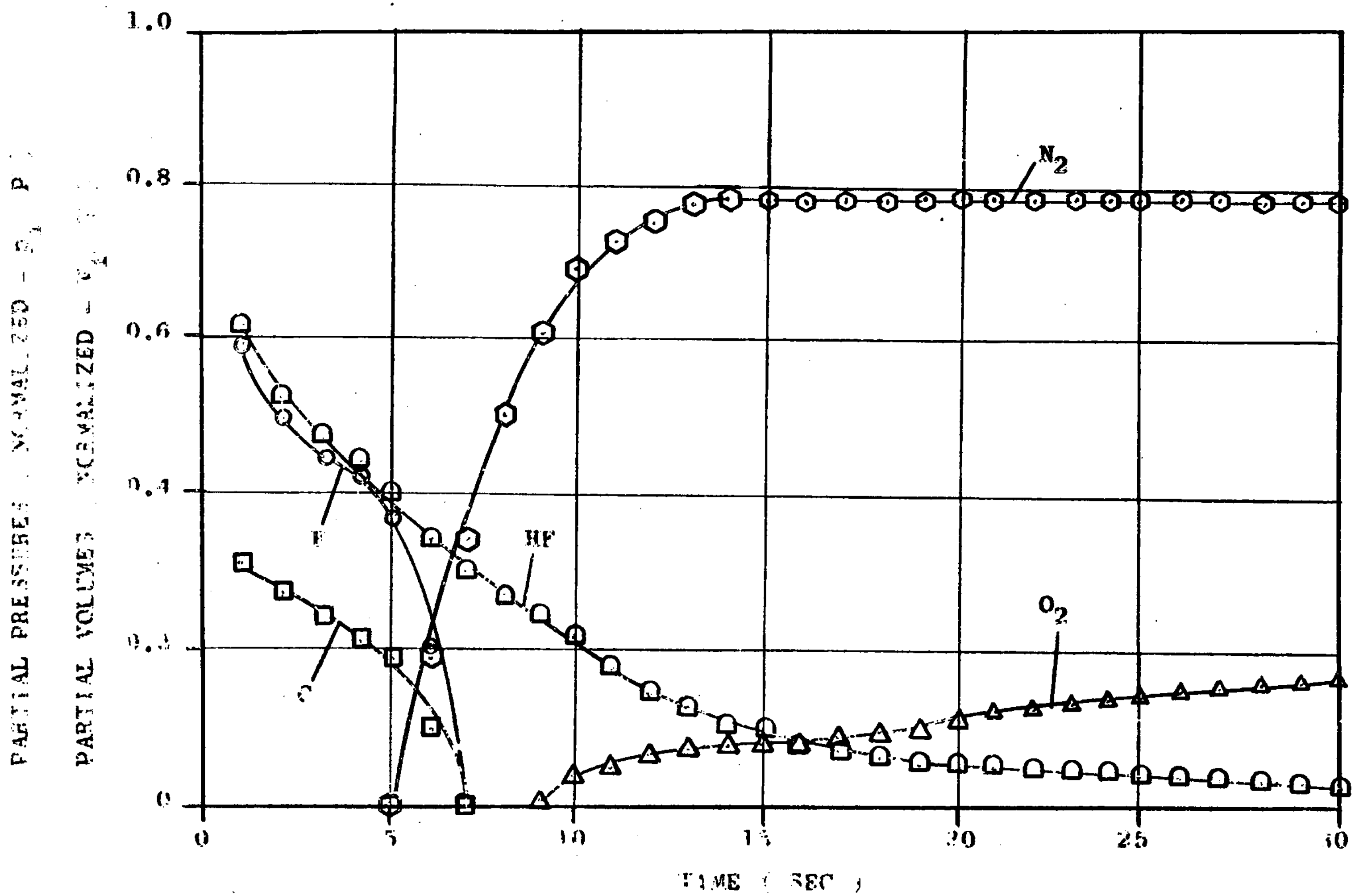


FIGURE 23-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR RP-1/LF$_2$ LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

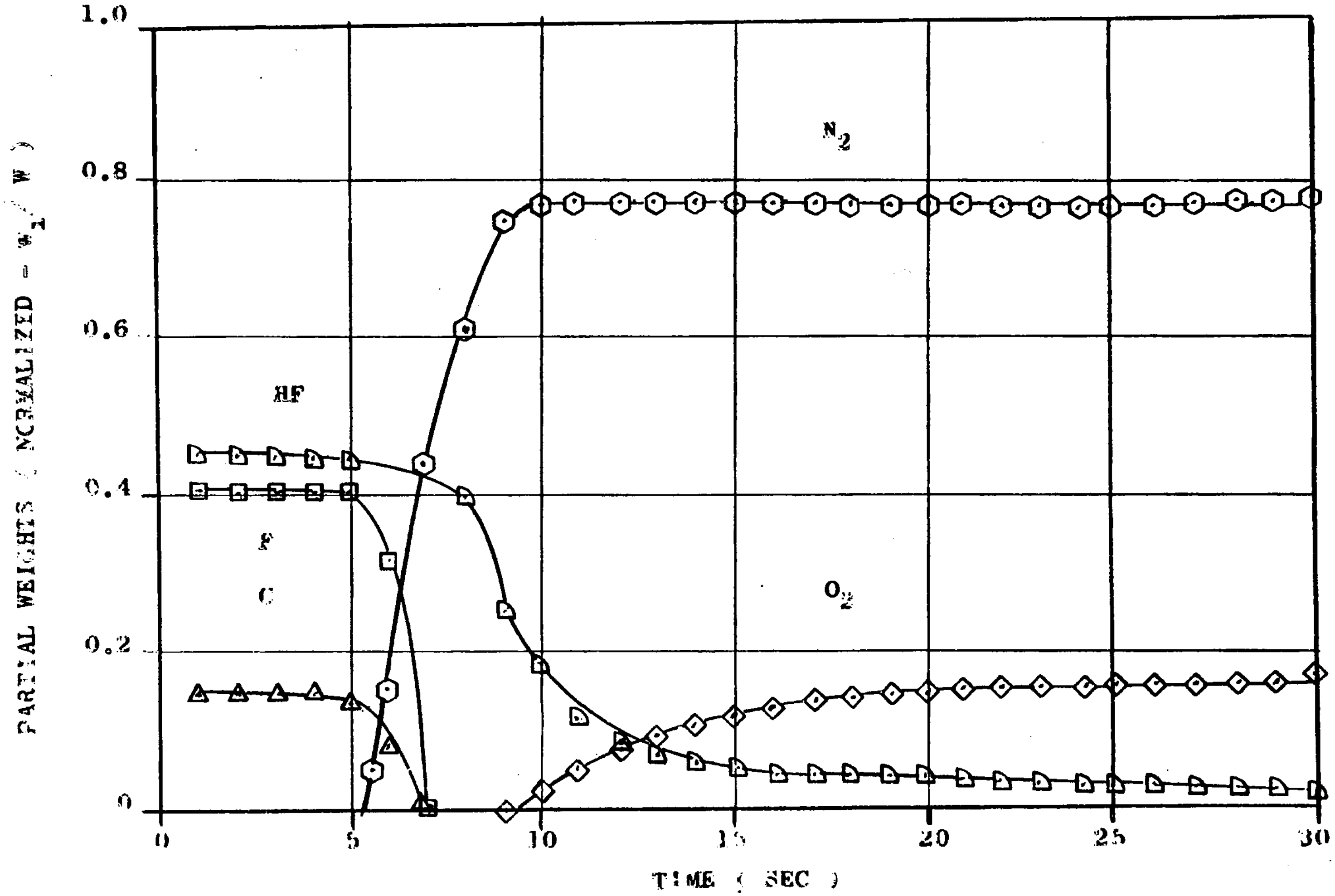


FIGURE 24. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM RP-1/LF_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

LH_2 / RP-1 / LO_2

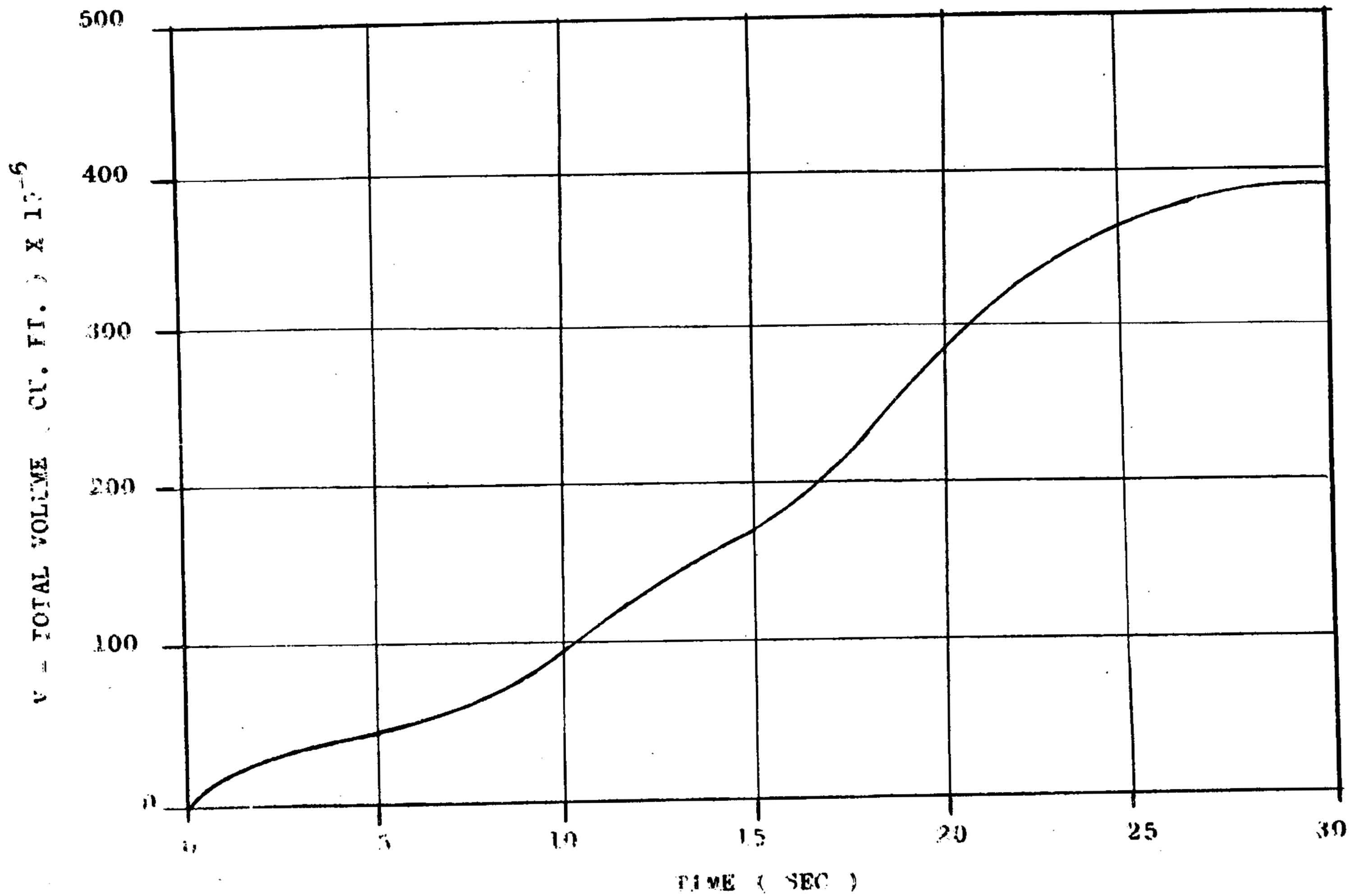


FIGURE 25. VOLUME TIME FUNCTION FOR LH_2/ RP-1/ LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD 4.5 PERCENT)

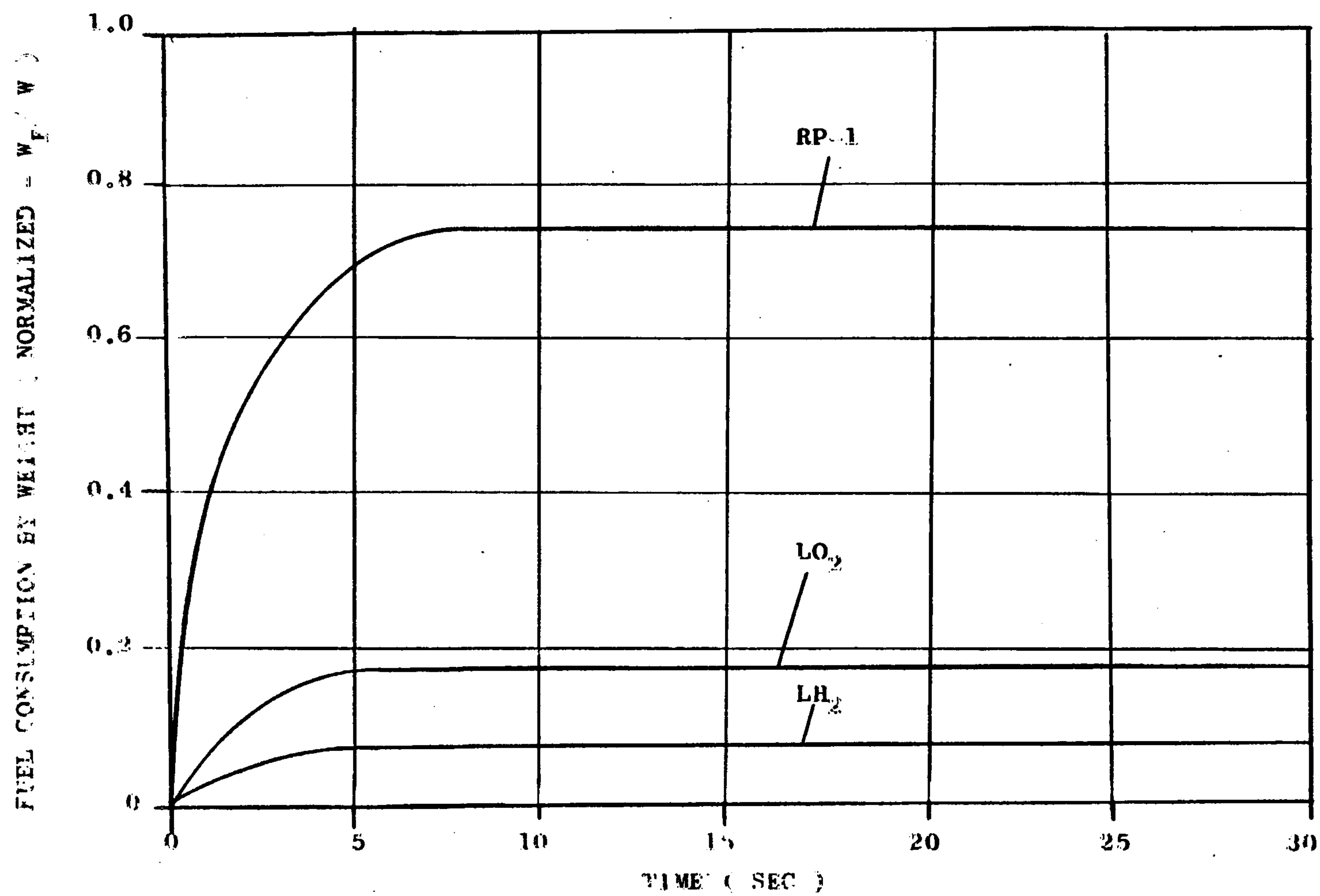


FIGURE 26. FUEL CONSUMPTION FOR LH_2/ RP-1/ LO_2 LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

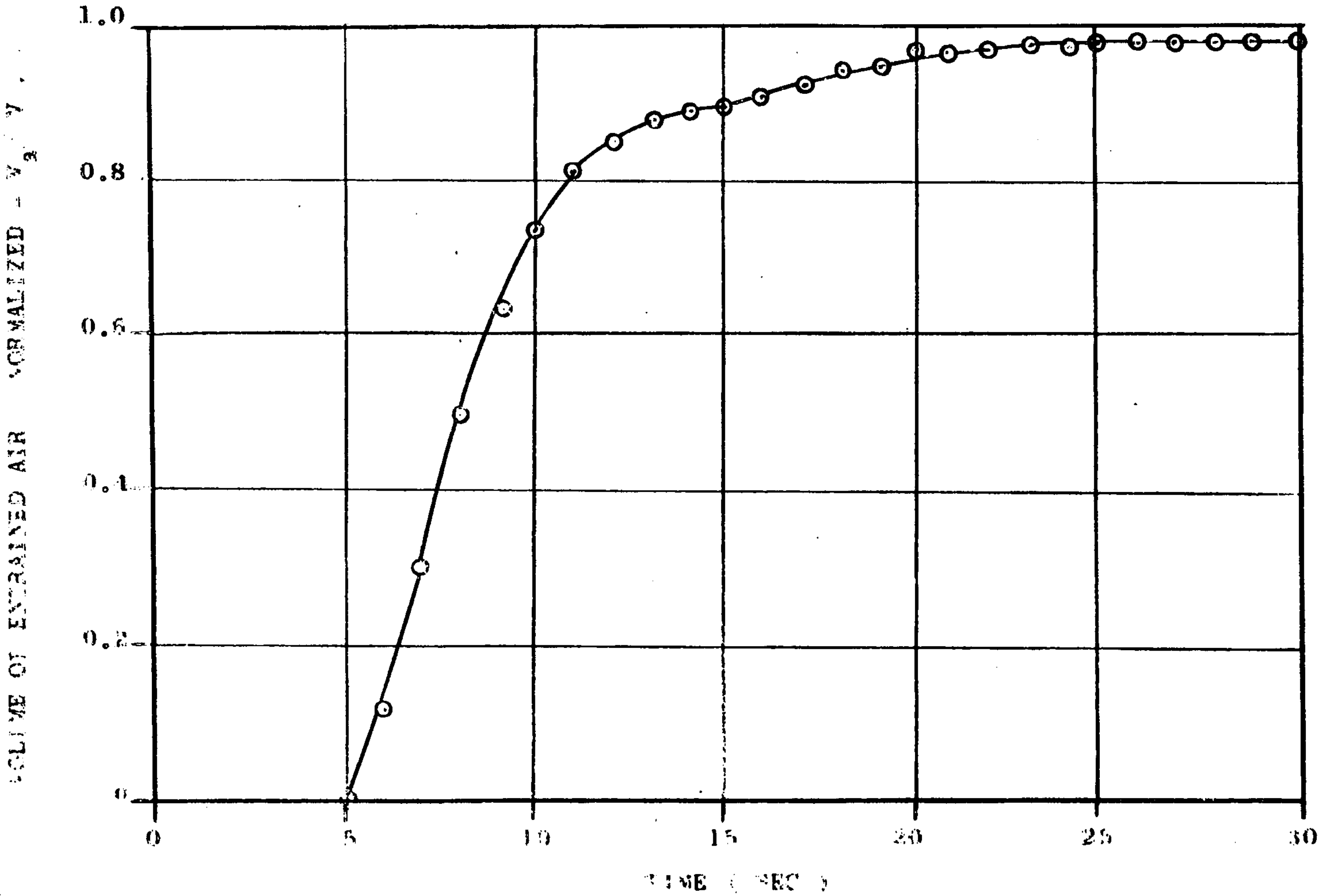


FIGURE 27. VOLUME OF ENTRAINED AIR FOR LH_2/RP-1/LO_2 LIQUID PROPELLANT EXPLOSION (YIELD ~ 3.5 PERCENT)

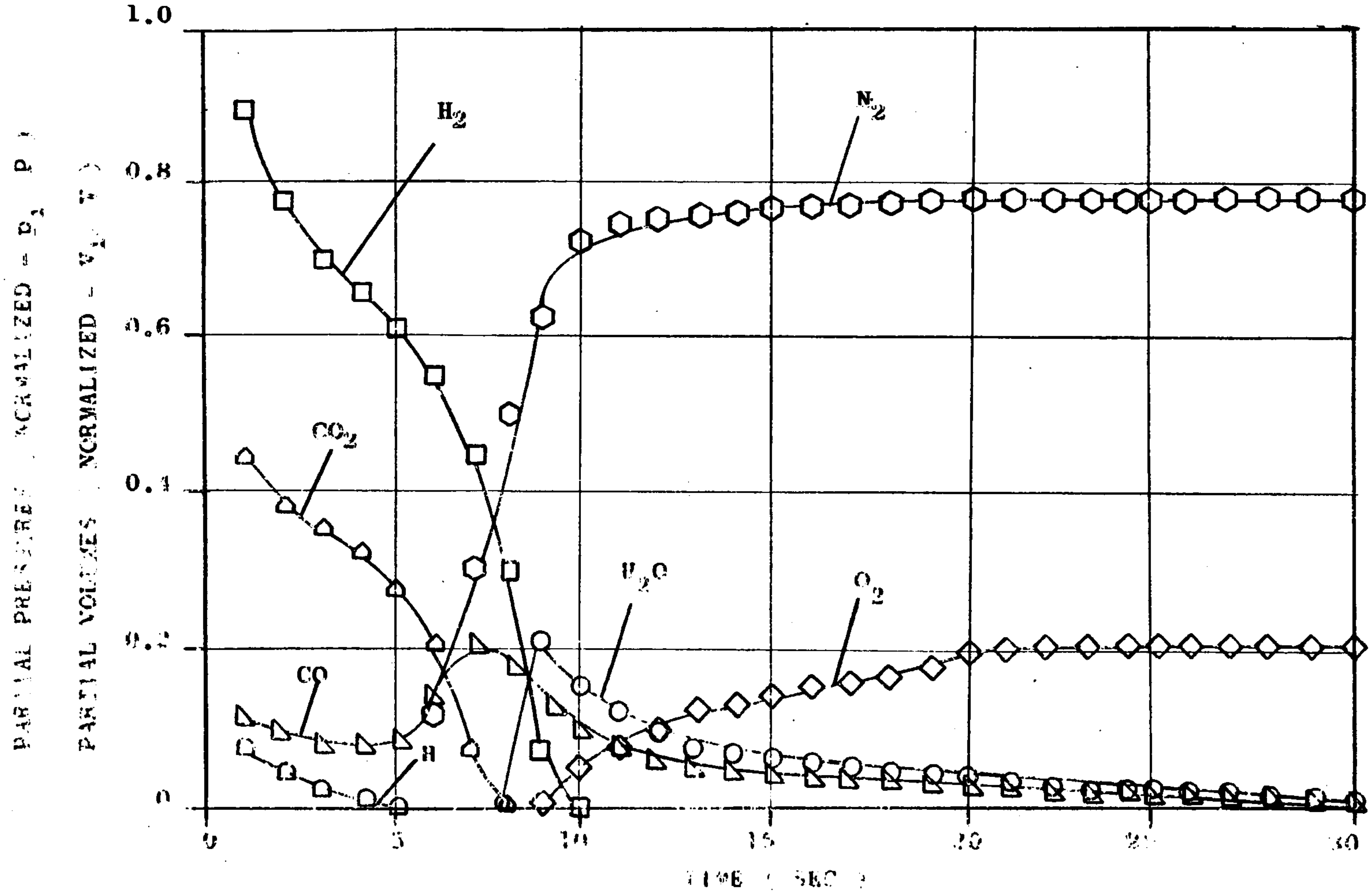


FIGURE 28 . PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/ RP-1/ LO_2 LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

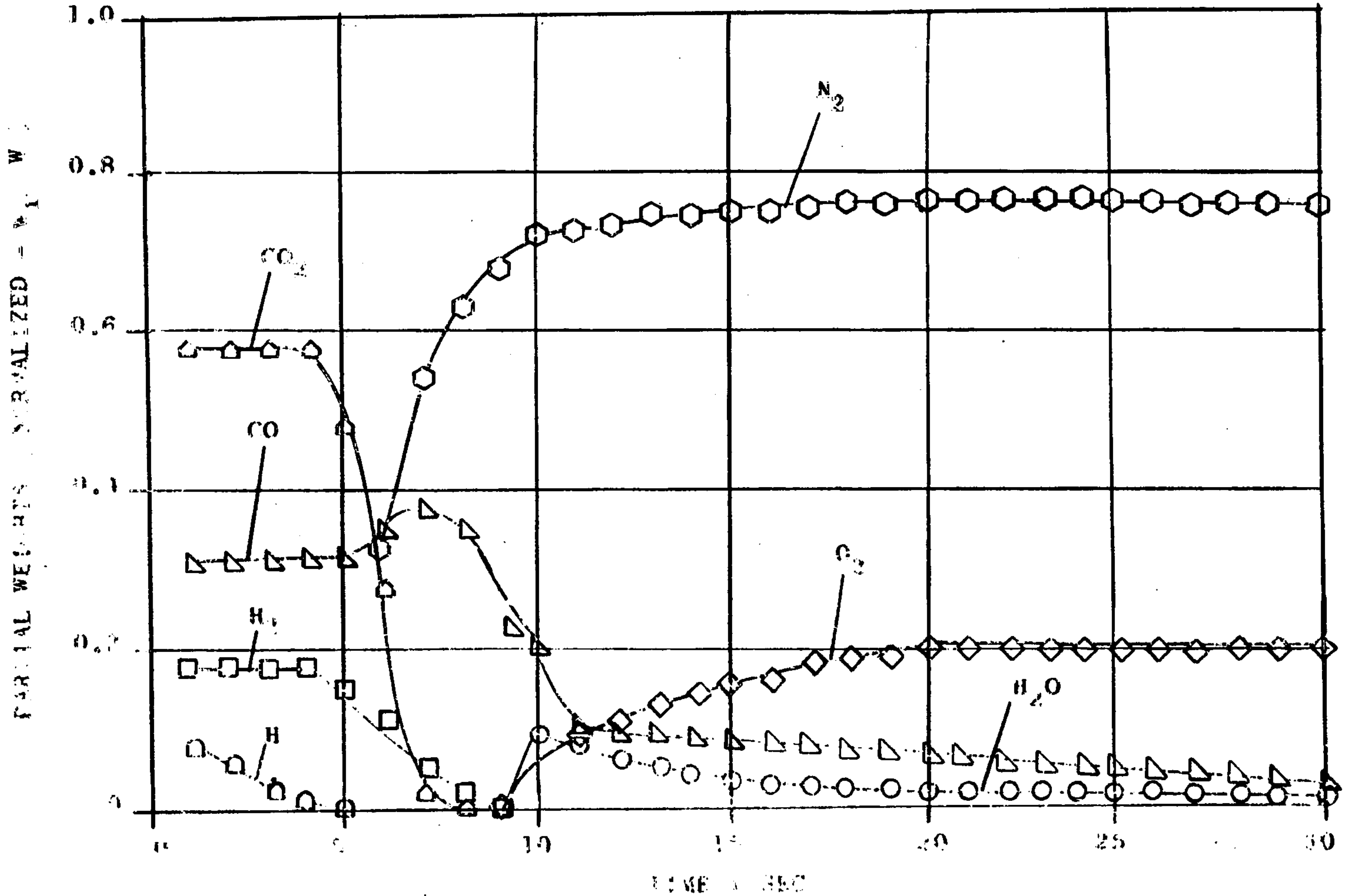


FIGURE 29 . WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LO_2 / RP-1 / LO_2

LIQUID PROPELLANT EXPLOSION (YIELD 4.5 PERCENT)

LH_2 / LO_2 - 1% F

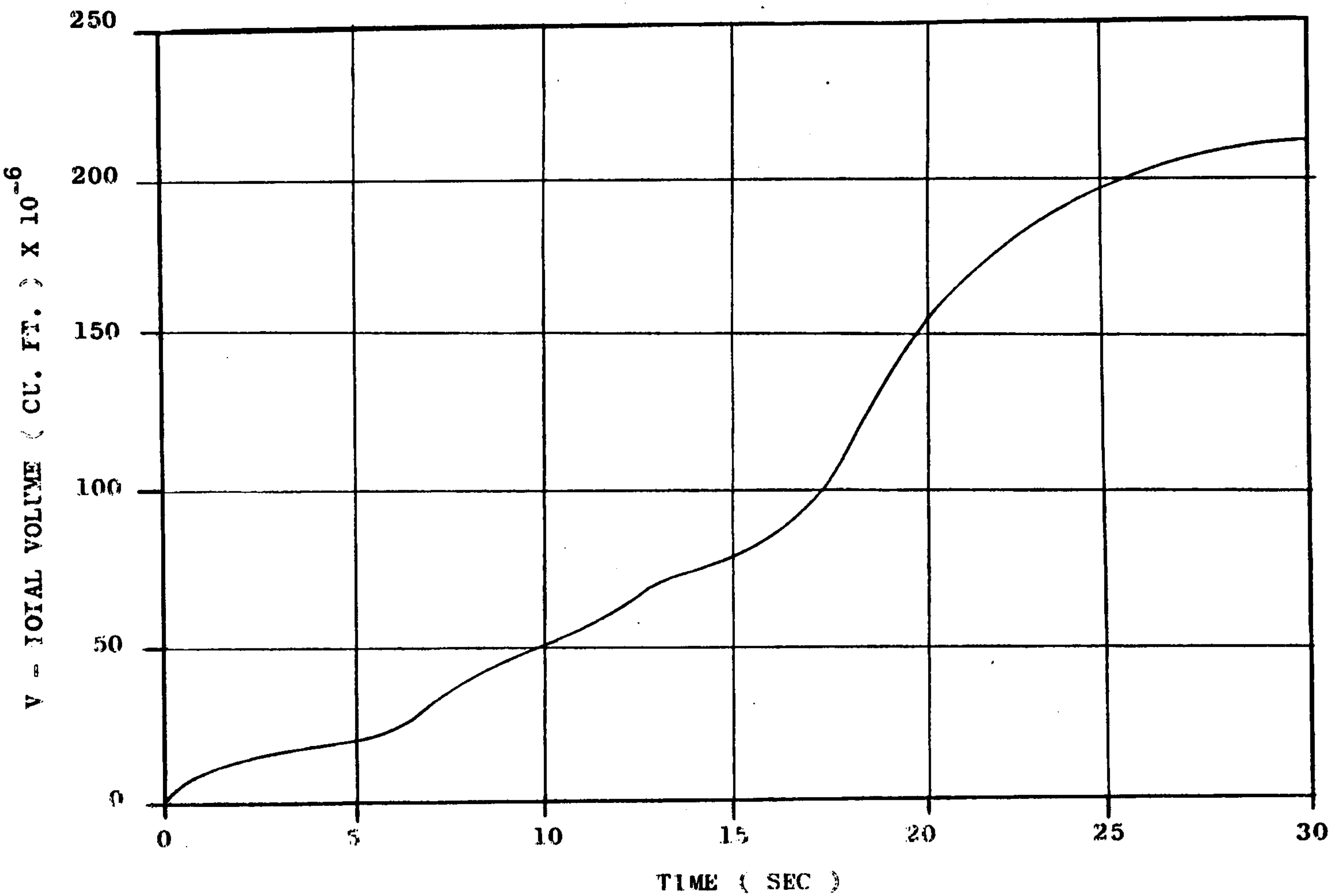


FIGURE 30-. VOLUME-TIME FUNCTION FOR LH_2/LO_2 + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 1.5 PERCENT)

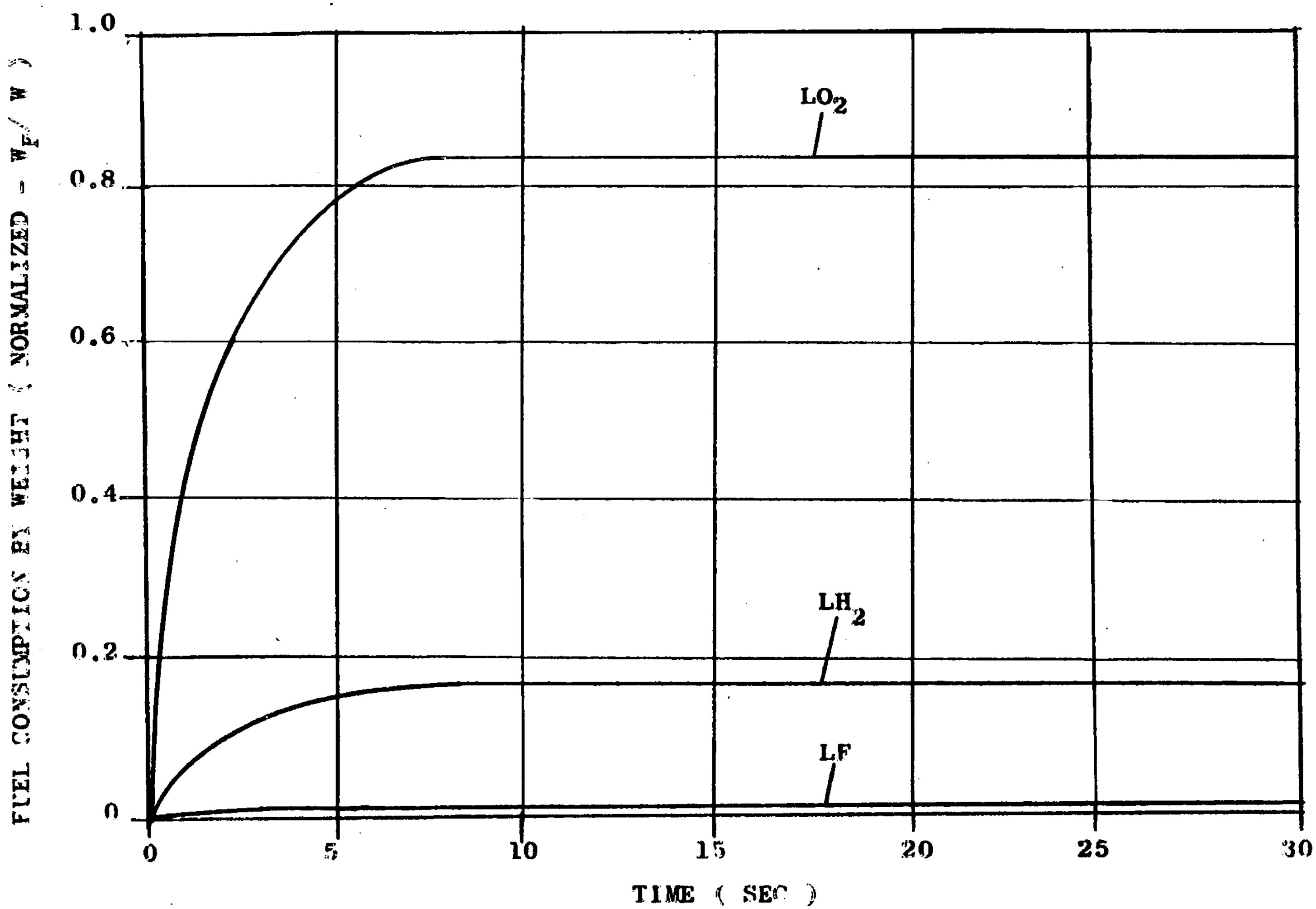


FIGURE 31-. FUEL CONSUMPTION FOR LH_2/LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

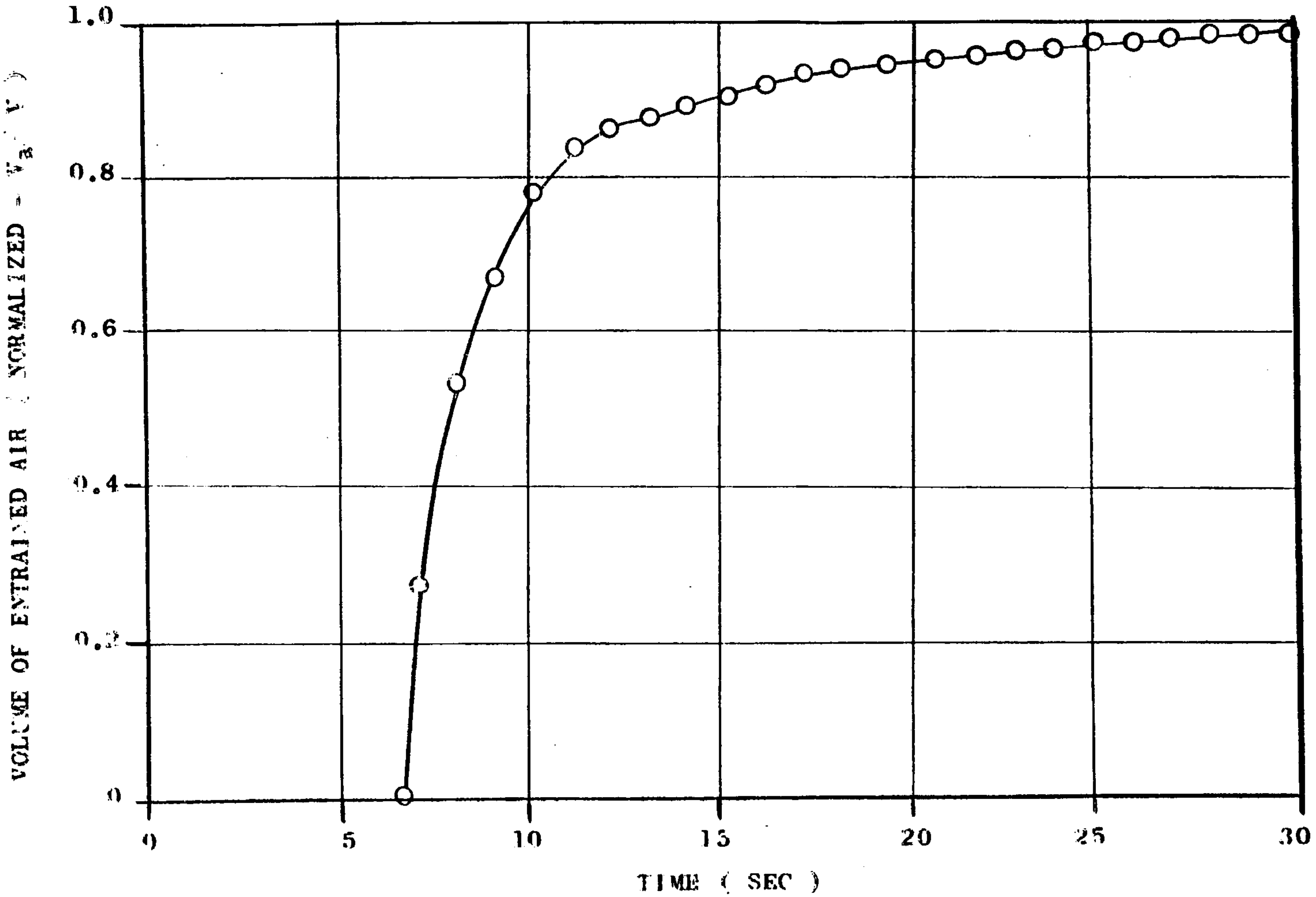


FIGURE 32-. VOLUME OF ENTRAINED AIR FOR LH_2/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD · 4.5 PERCENT)

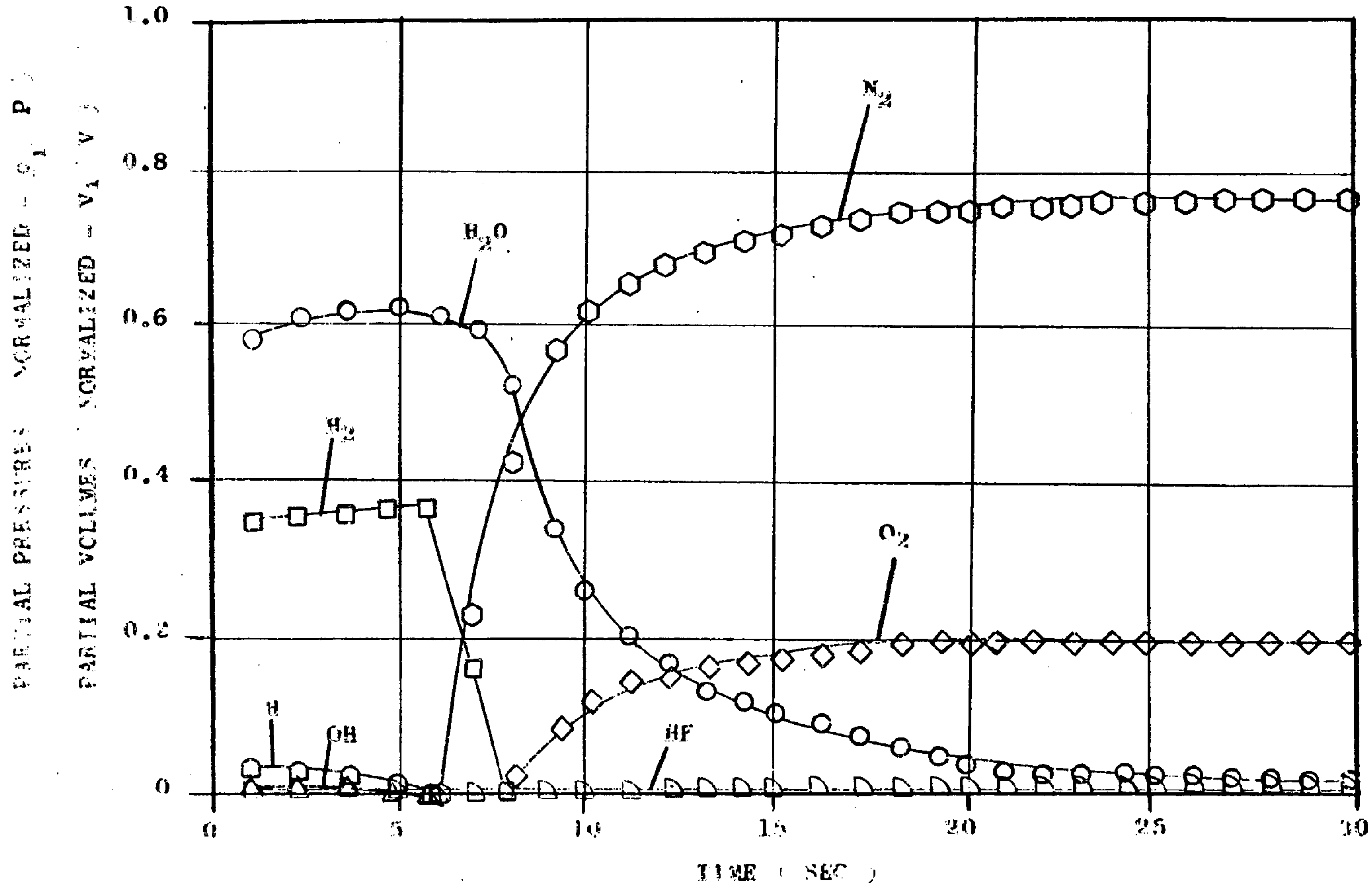


FIGURE 33-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

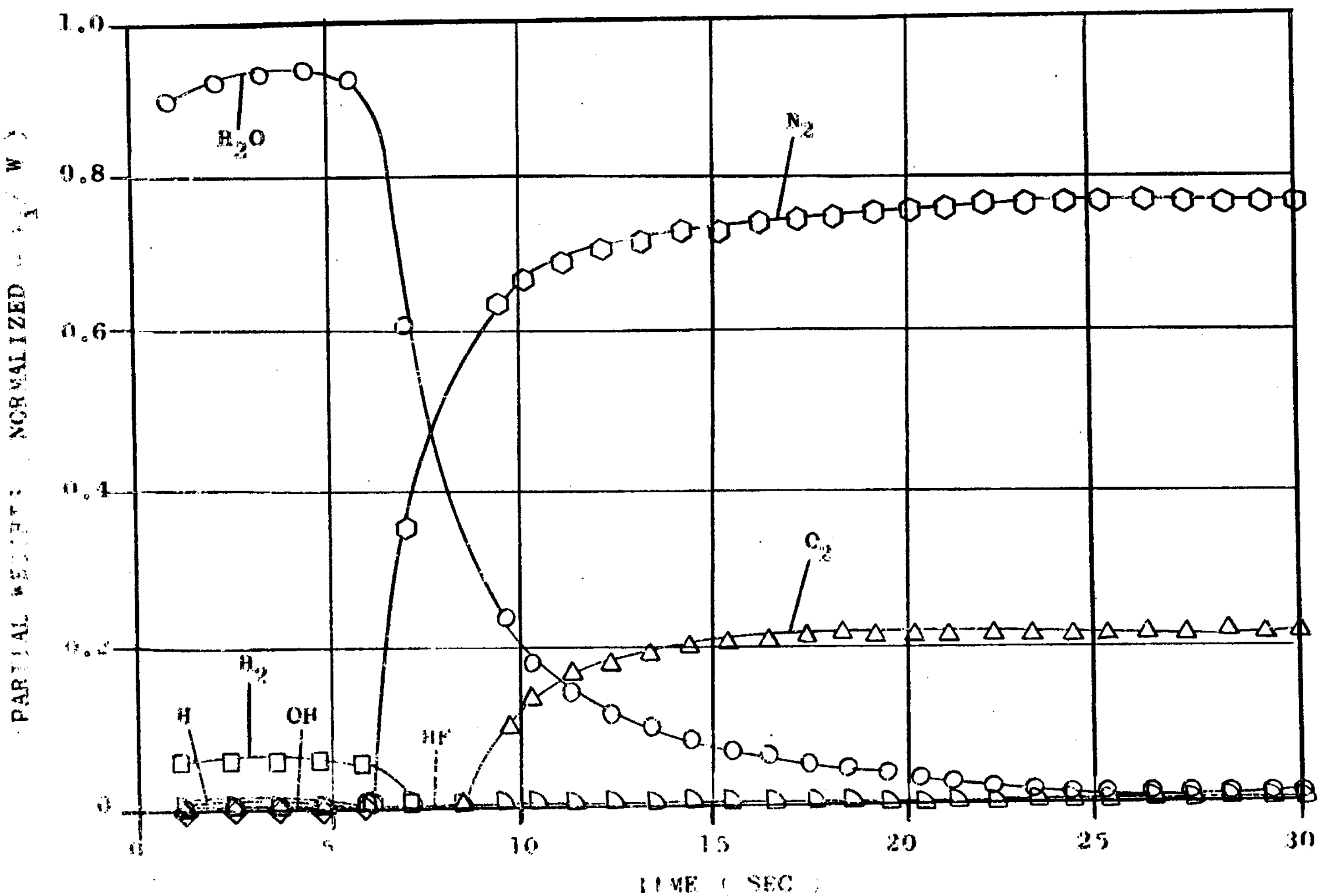


FIGURE [illegible]. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/ LO_2 + 1%F

LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

LH_2 / LO_2 - 5% F

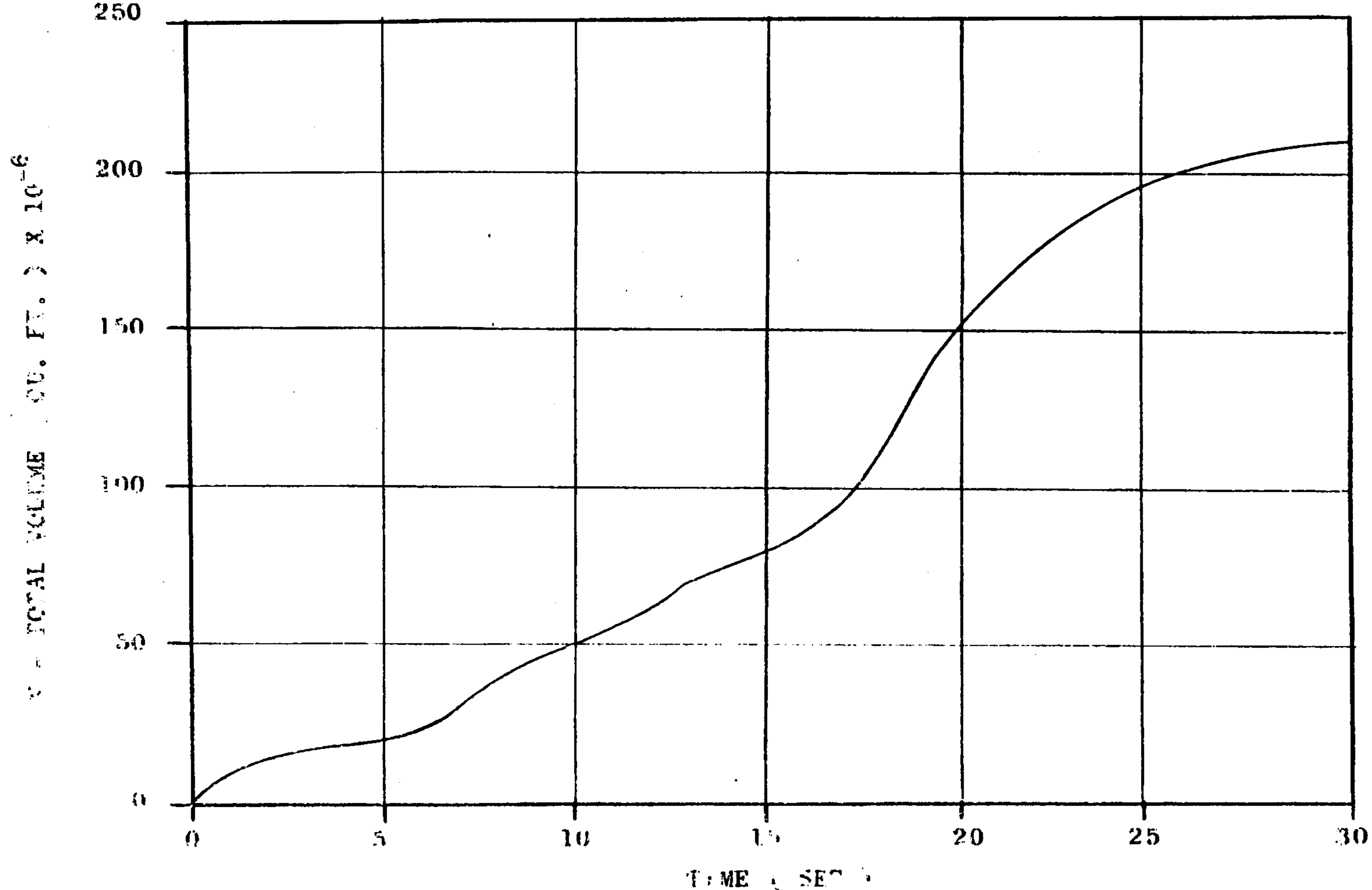


FIGURE (5-), VOLUME-TIME FUNCTION FOR LH_2/ LO_2 + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

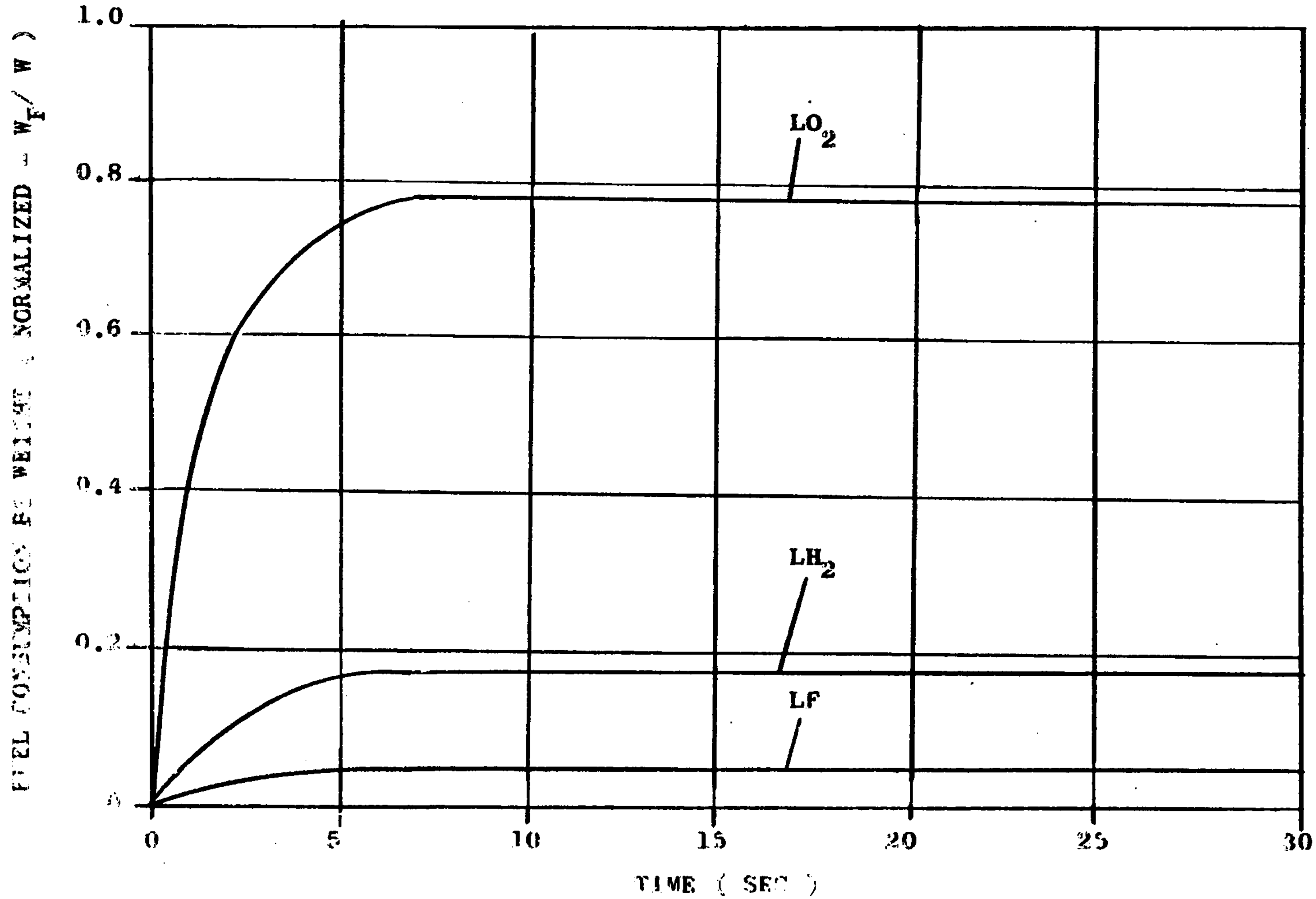


FIGURE 36[illegible]. FUEL CONSUMPTION FOR LH_2/LO_2 + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

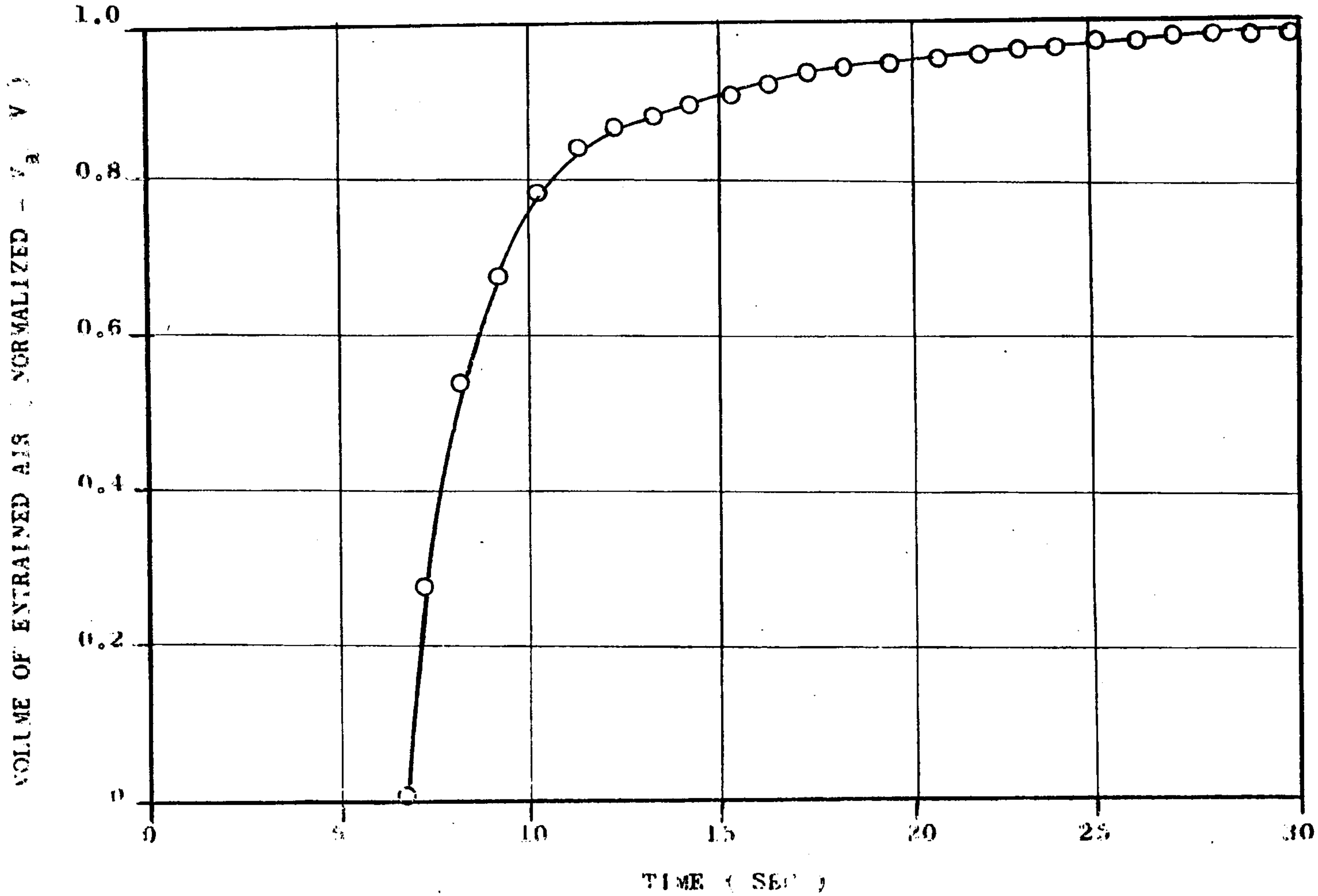


FIGURE 37. VOLUME OF ENTRAINED AIR FOR LH_2/LO_2 + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 1.5 PERCENT)

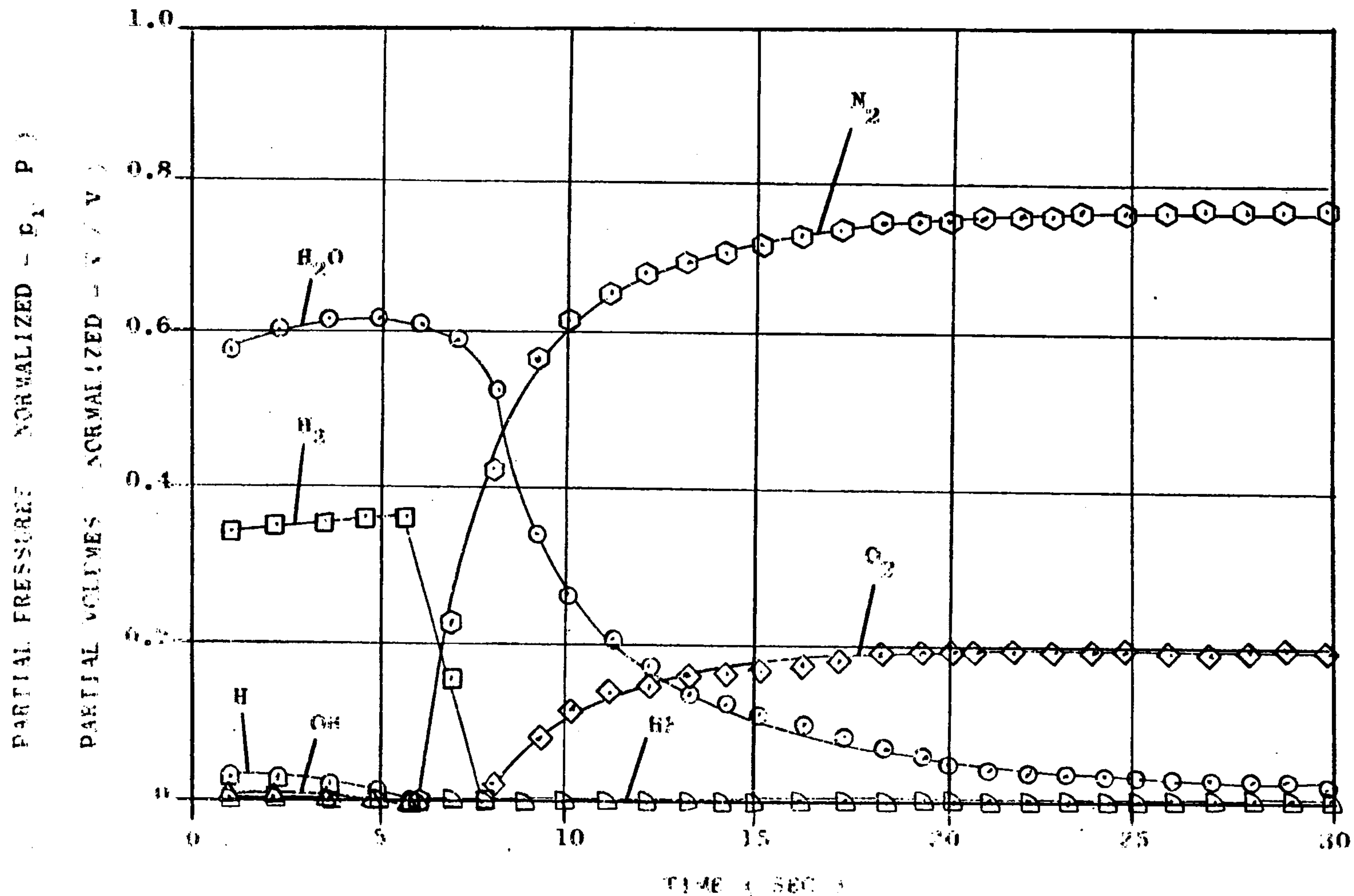


FIGURE 38-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/ LO_2 + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

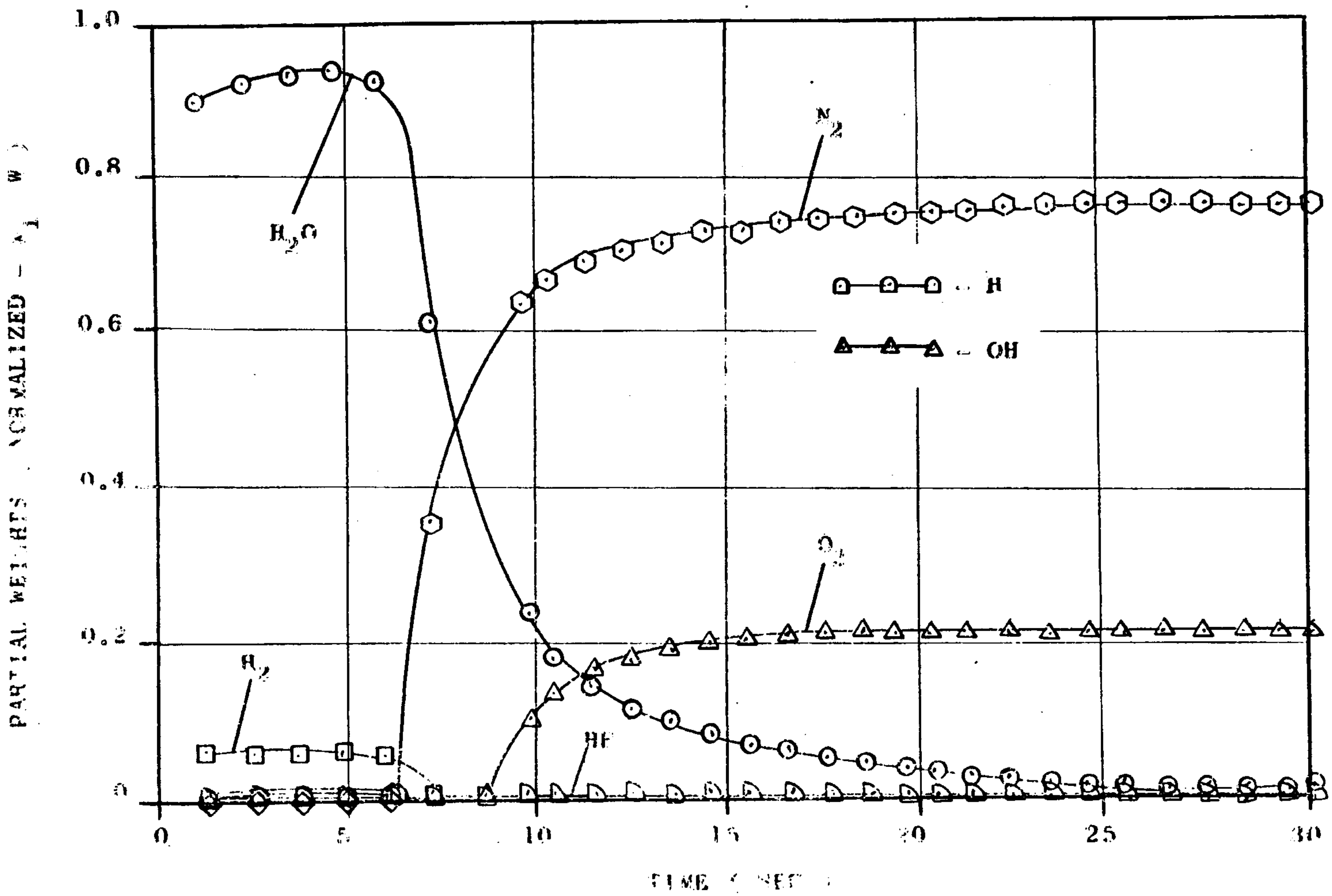


FIGURE 19-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/ LO_2 + 5% F

LIQUID PROPELLANT EXPLOSION (YIELD - 4.5 PERCENT)

LH_2 / LO_2 + 10% F

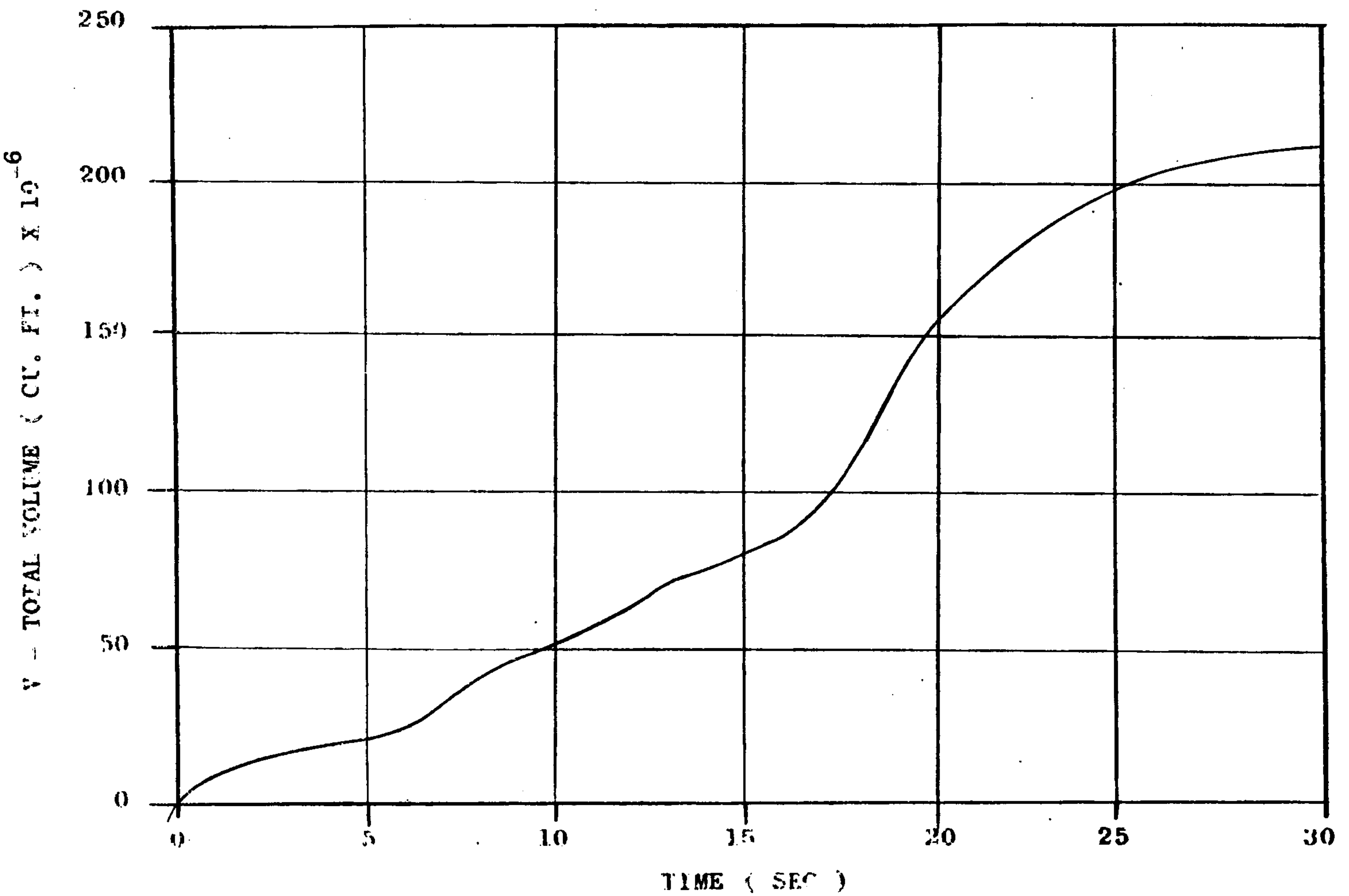


FIGURE 40-. VOLUME-TIME FUNCTION FOR LH_2/ LO_2 + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

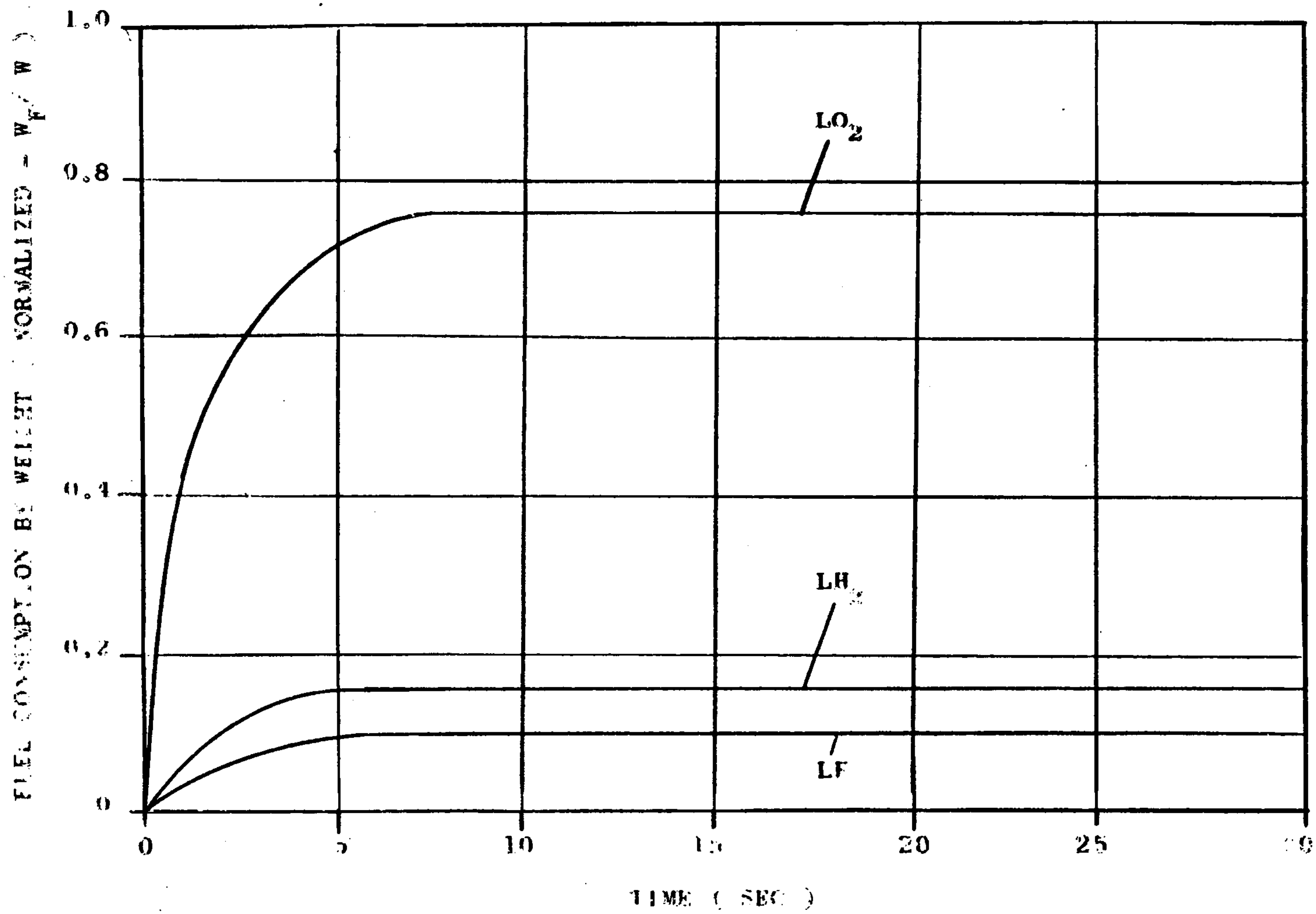


FIGURE 41. FUEL CONSUMPTION FOR LH_2, LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD ≈ 4.5 PERCENT)

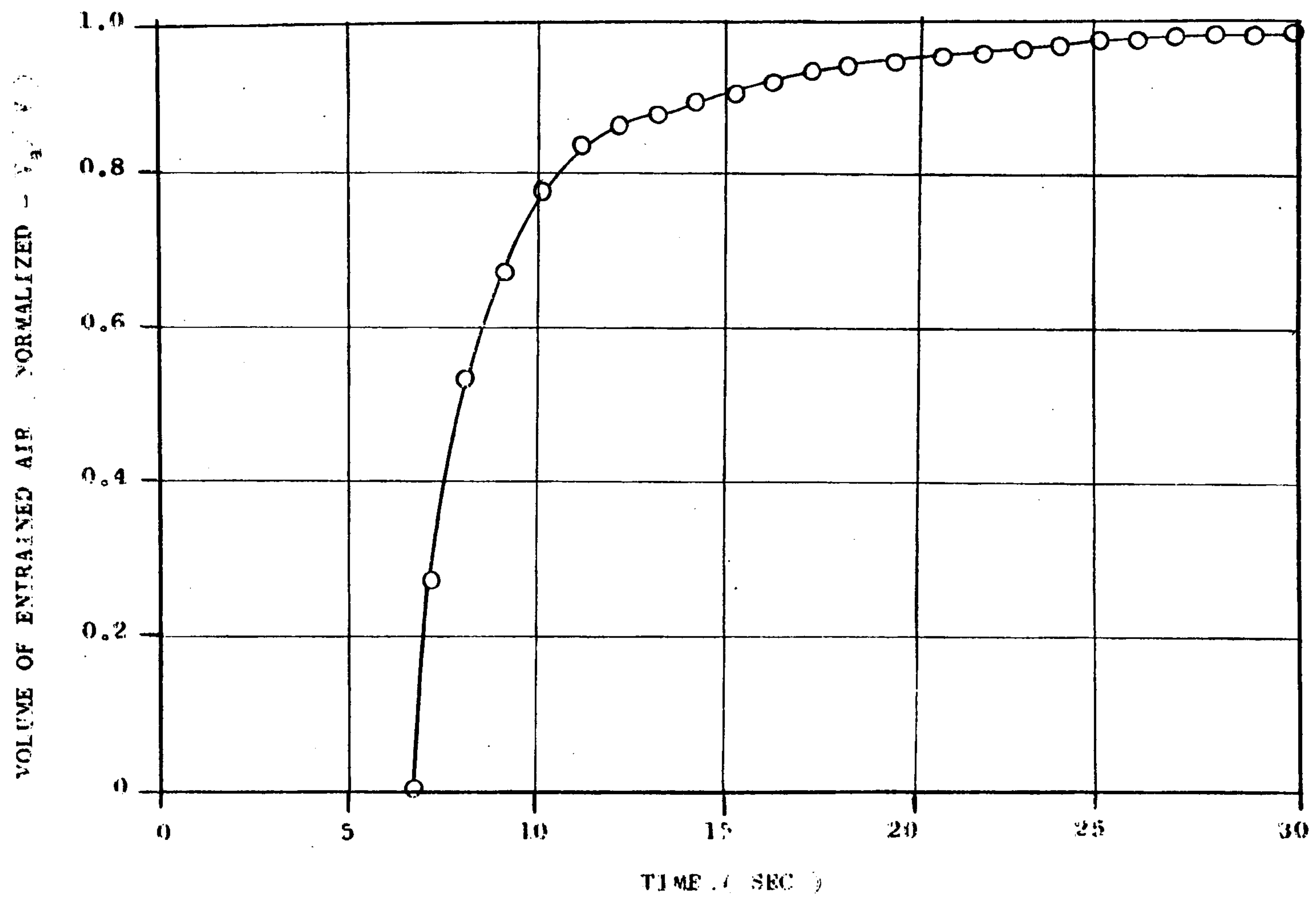


FIGURE 42-, VOLUME OF ENTRAINED AIR FOR LH_2 / LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

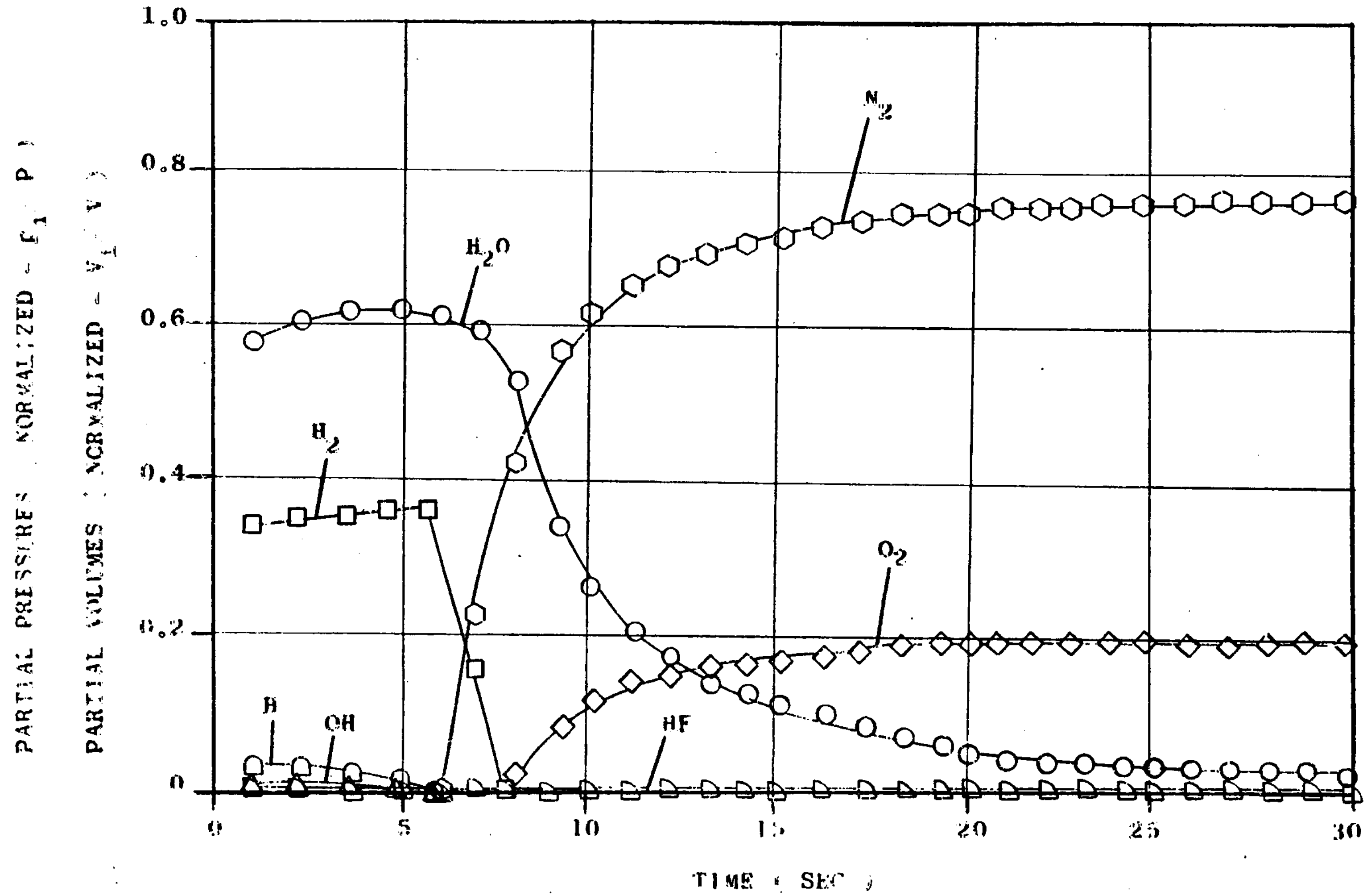


FIGURE 43 . PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/ LO_2 + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

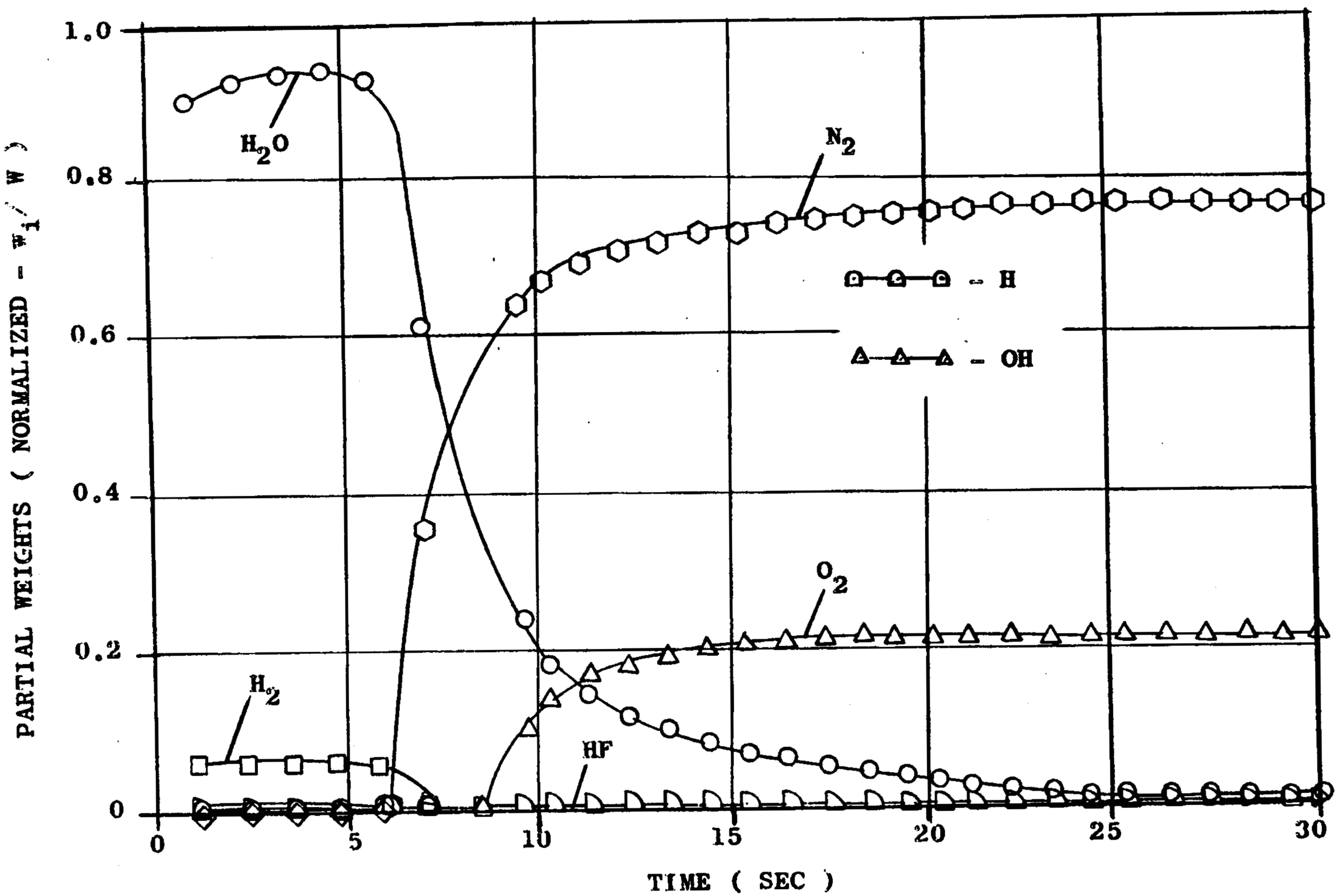


FIGURE 44-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/ LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

RP-1 / LO_2 + 1% F

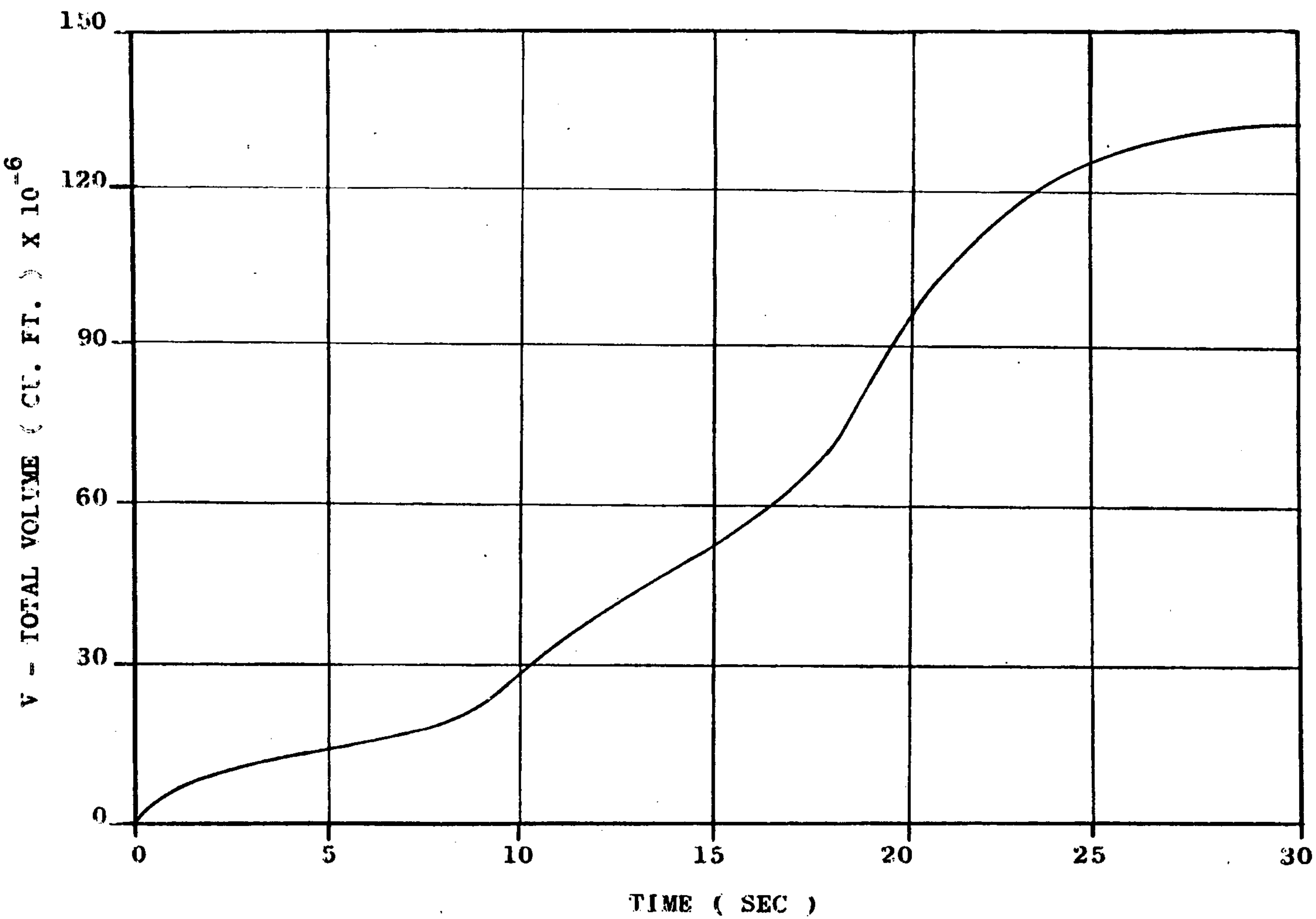


FIGURE 45-. VOLUME-TIME FUNCTION FOR RP-1/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD ~ 4.5 PERCENT)

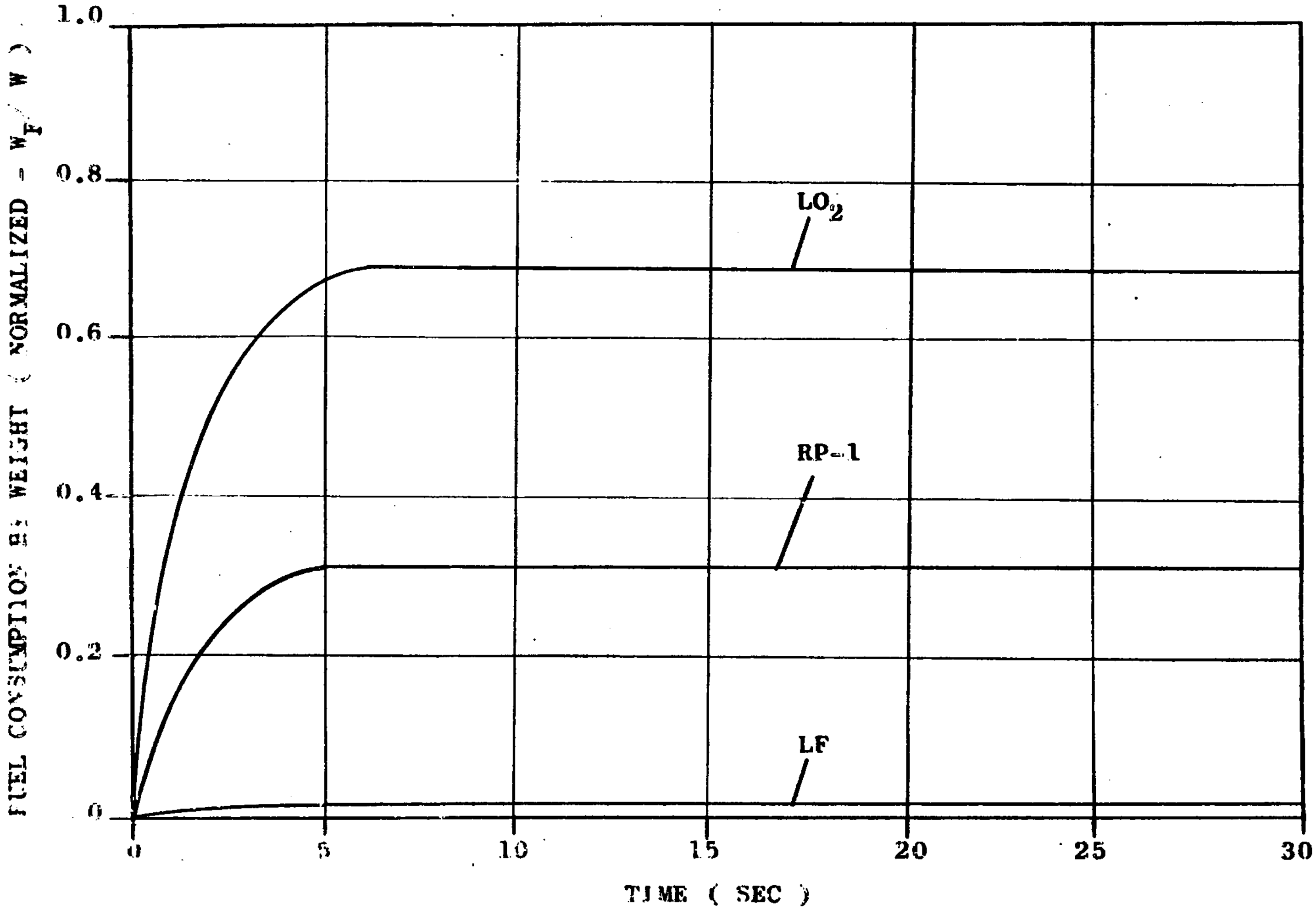


FIGURE 46-. FUEL CONSUMPTION FOR RP-1/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

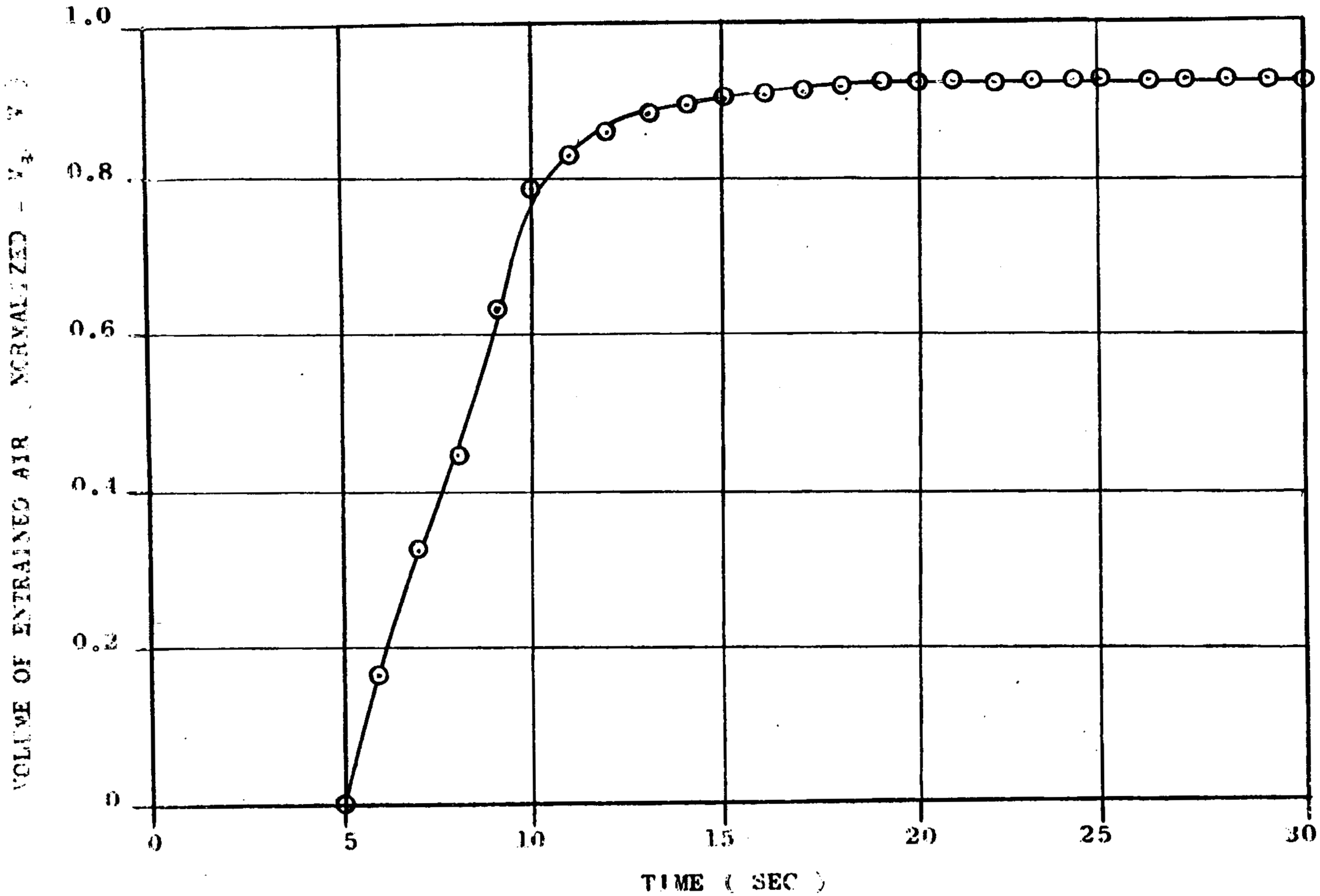


FIGURE 47-. VOLUME OF ENTRAINED AIR FOR RP 1/LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

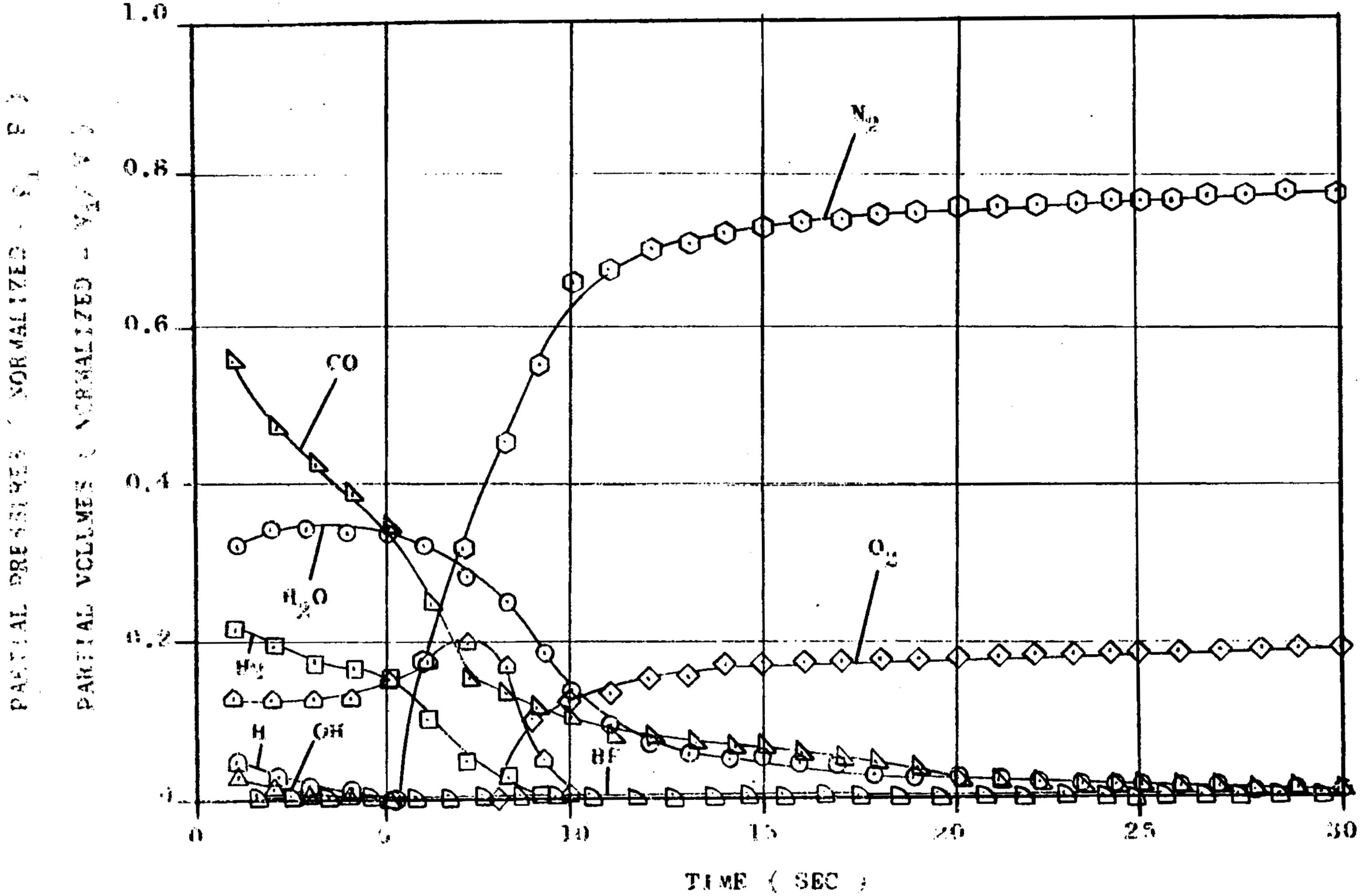


FIGURE 48-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR RP-1/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

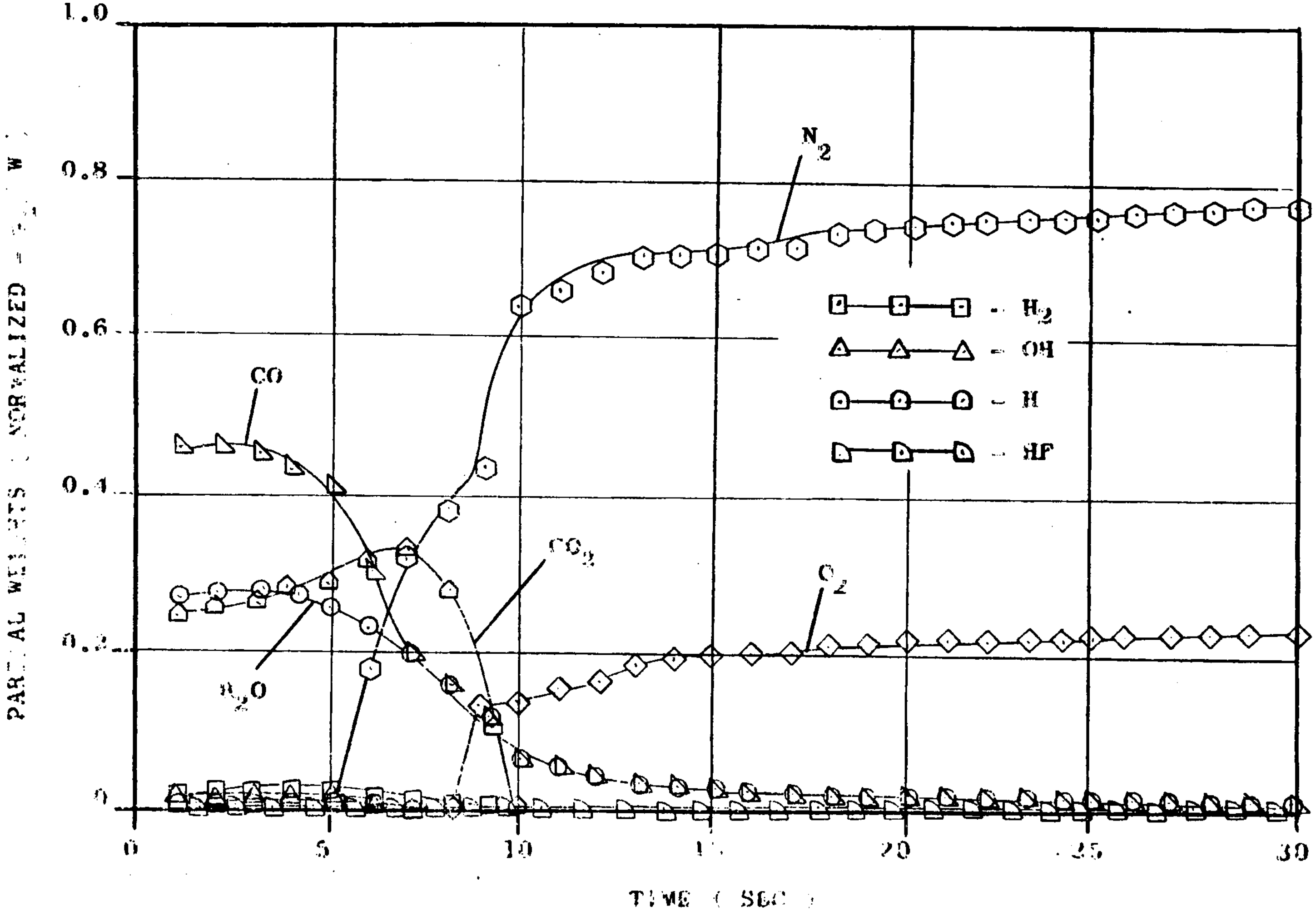


FIGURE 49 . WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM RP-1/ LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

RP-1 / LO_2 + 5% F

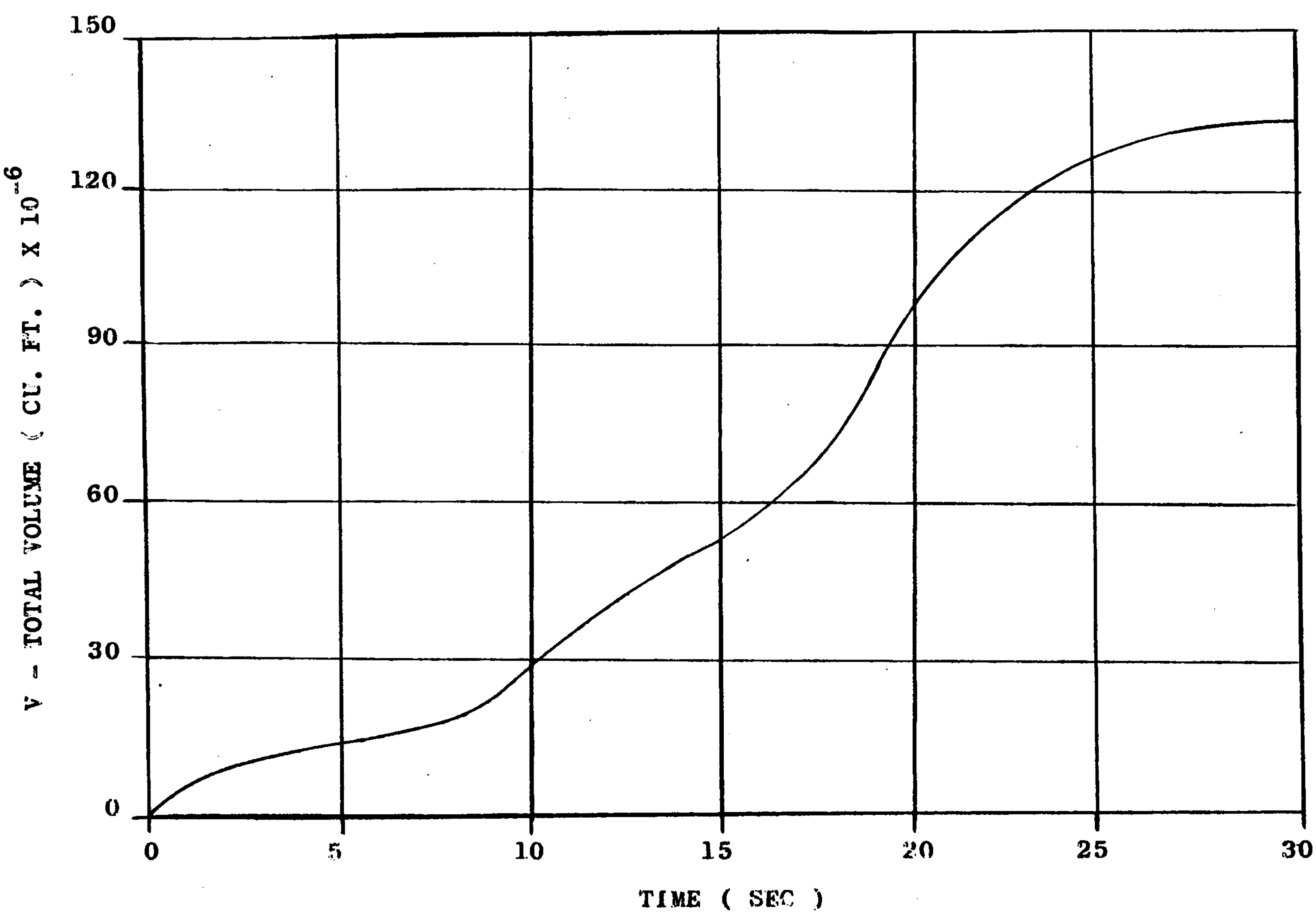


FIGURE 50-. VOLUME-TIME FUNCTION FOR RP-1/ LO_2 + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

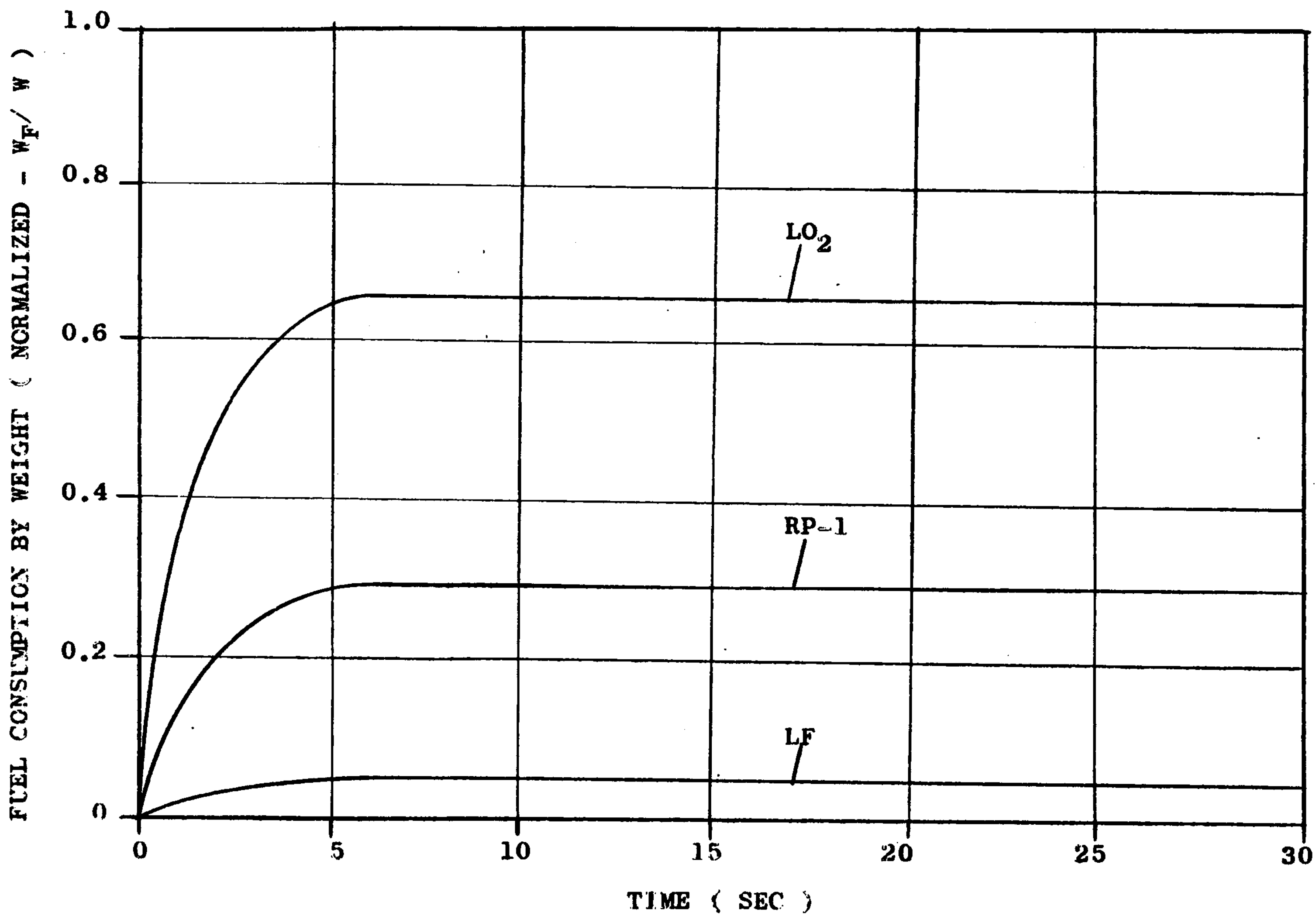


FIGURE 51-. FUEL CONSUMPTION FOR RP-1/ LO_2 + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

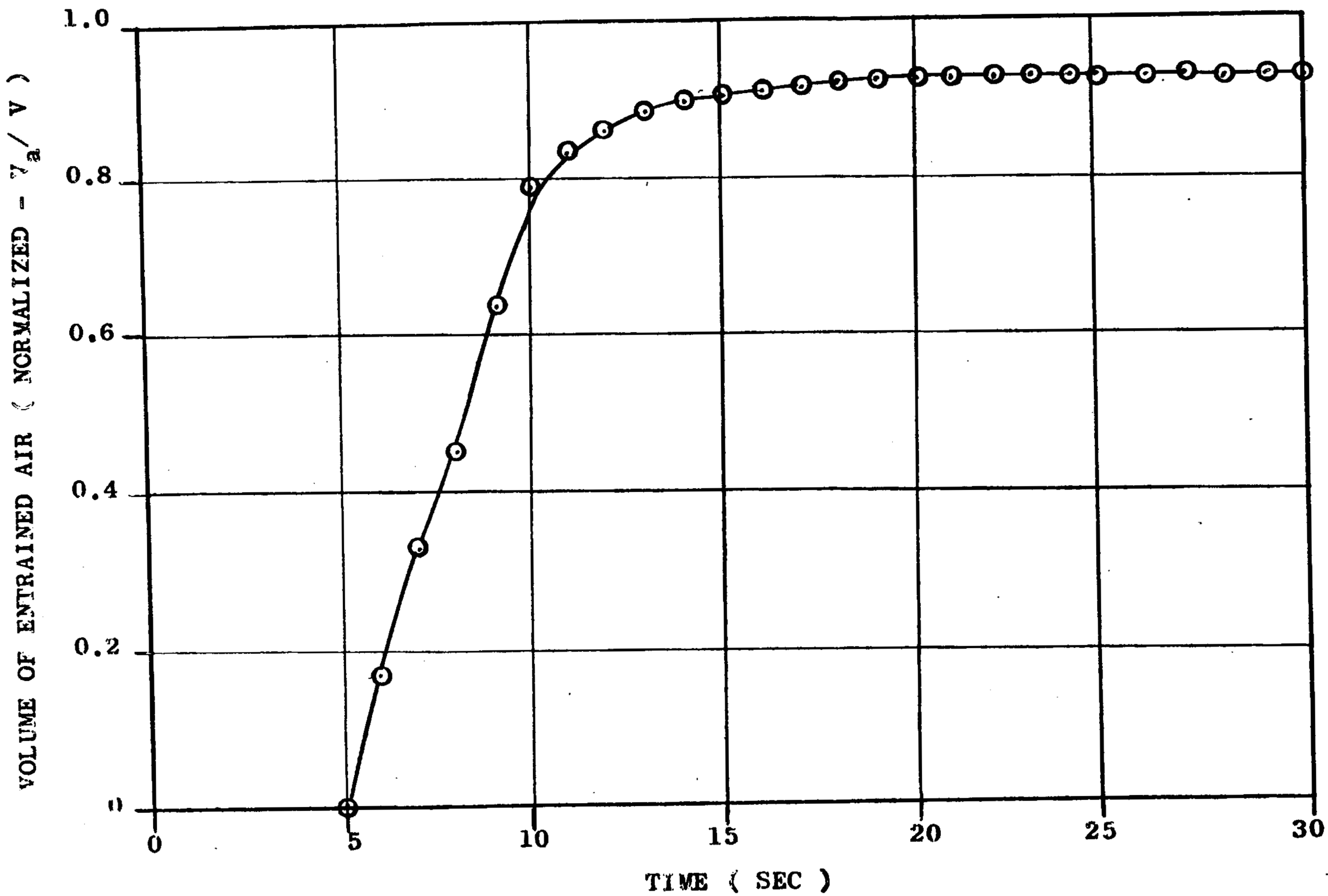


FIGURE 52-. VOLUME OF ENTRAINED AIR FOR RP-1/LO_2 + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

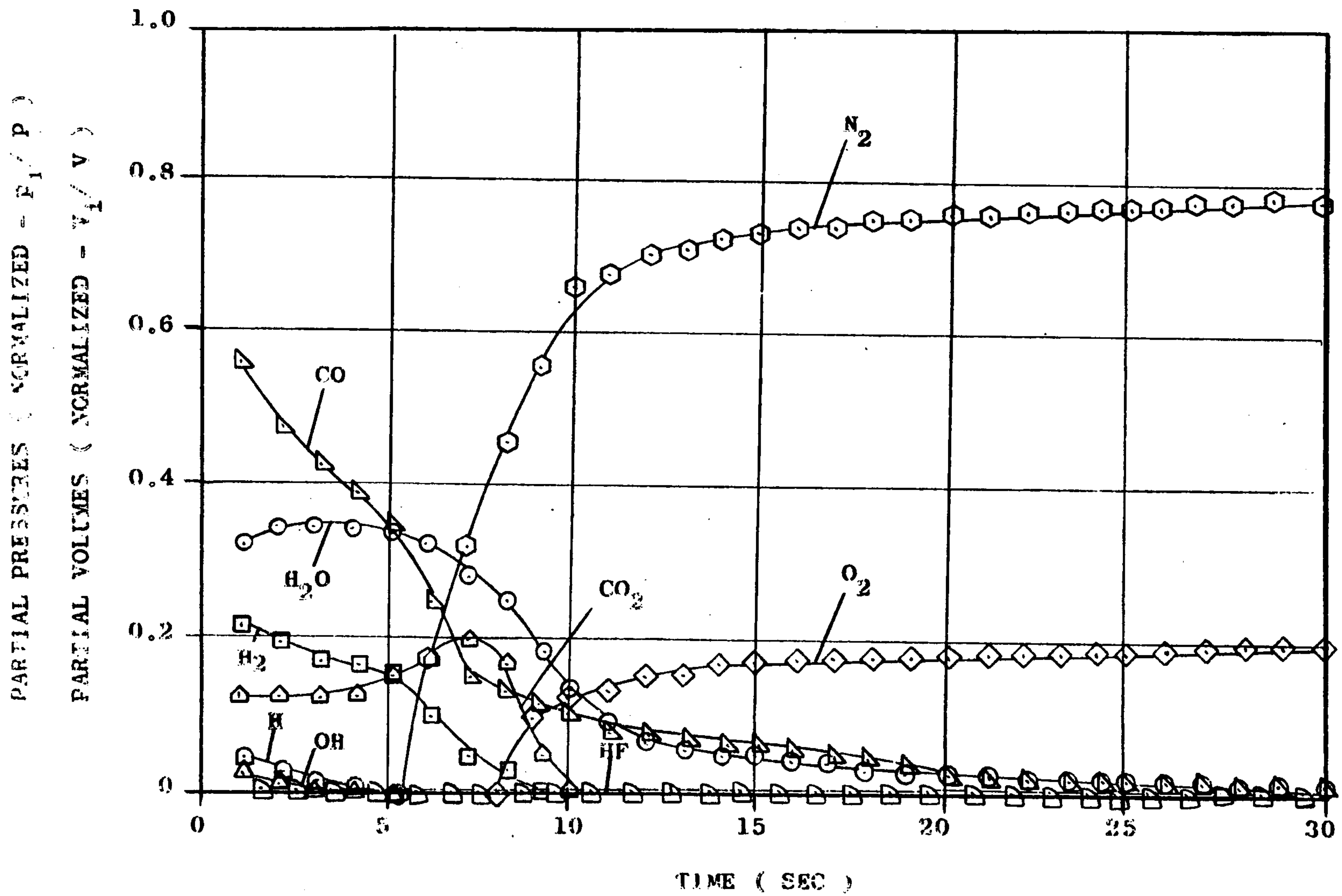


FIGURE 53-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR RP-1/ LO_2 + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

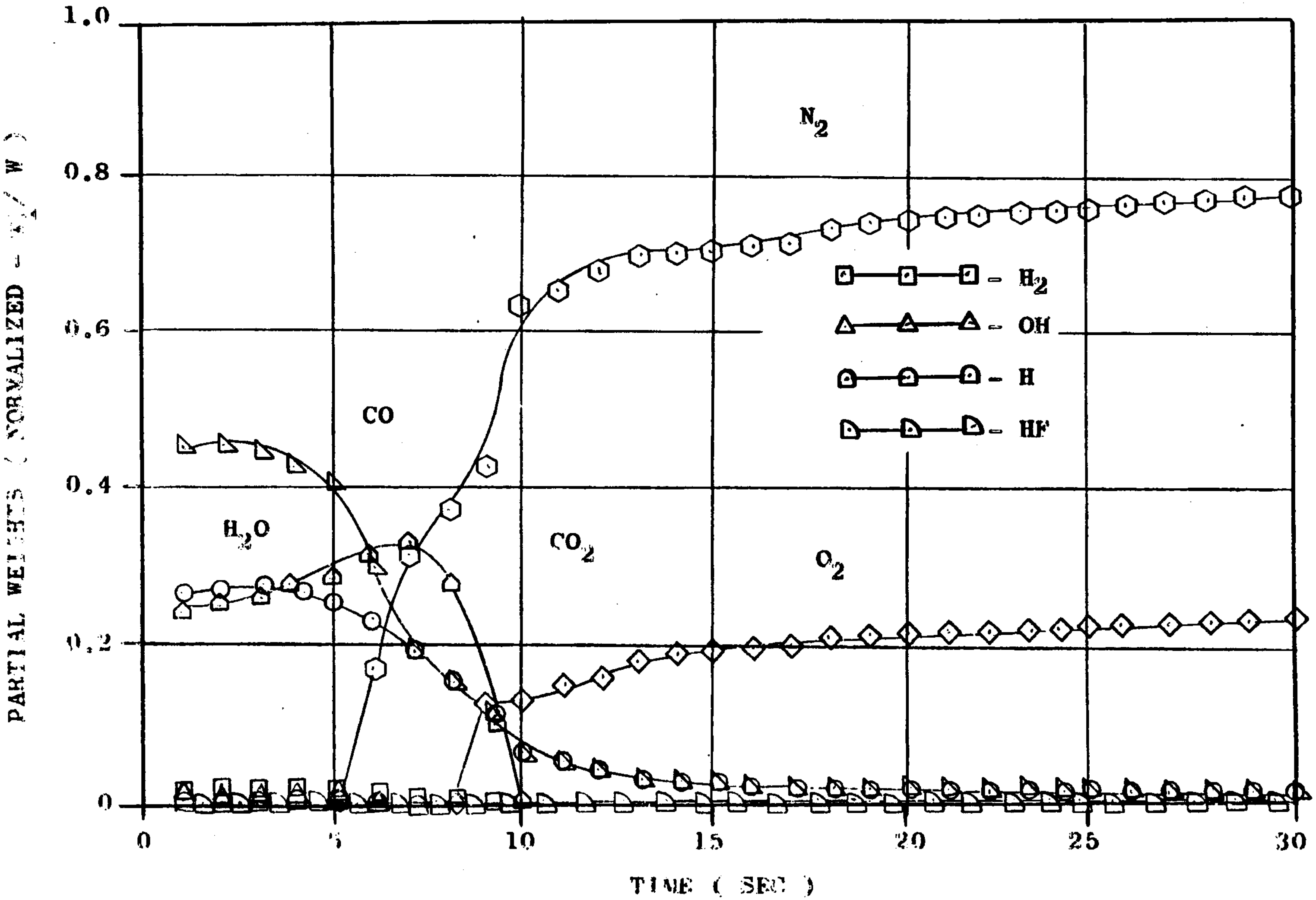


FIGURE 54. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM RP-1/LO_2+ 5%F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

RP-1 / LO_2 + 10% F

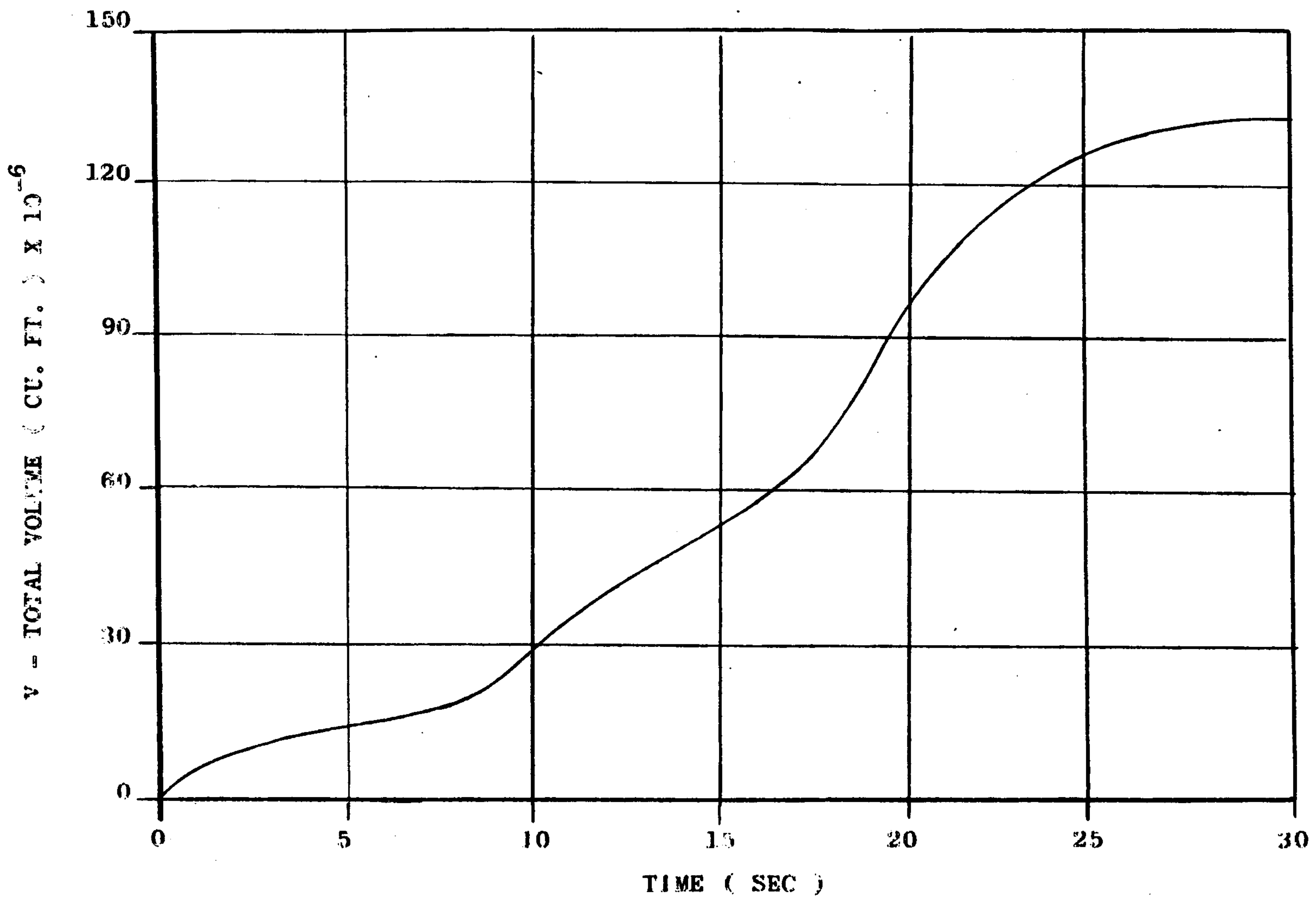


FIGURE 55-. VOLUME-TIME FUNCTION FOR RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

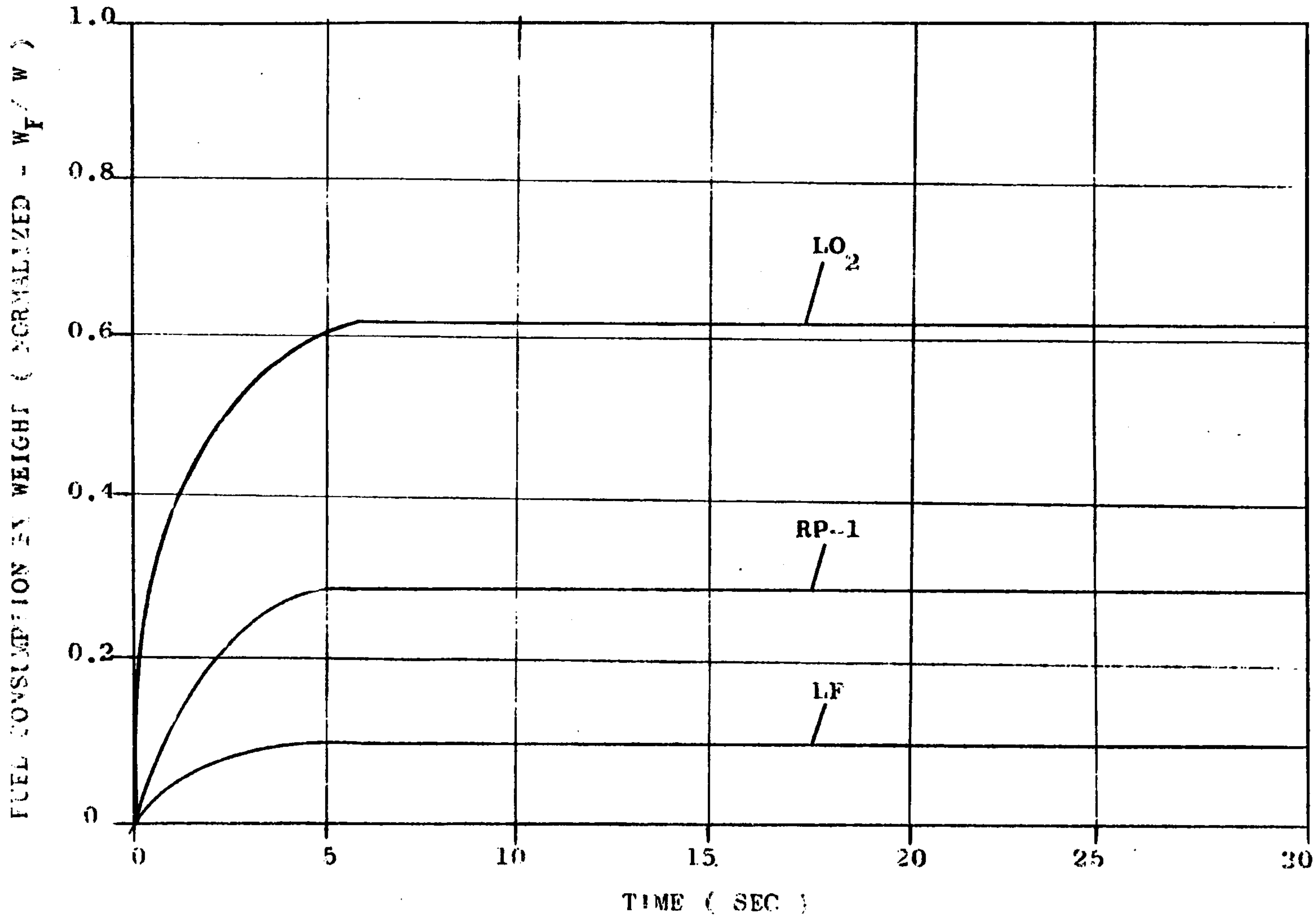


FIGURE 56-. FUEL CONSUMPTION FOR RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

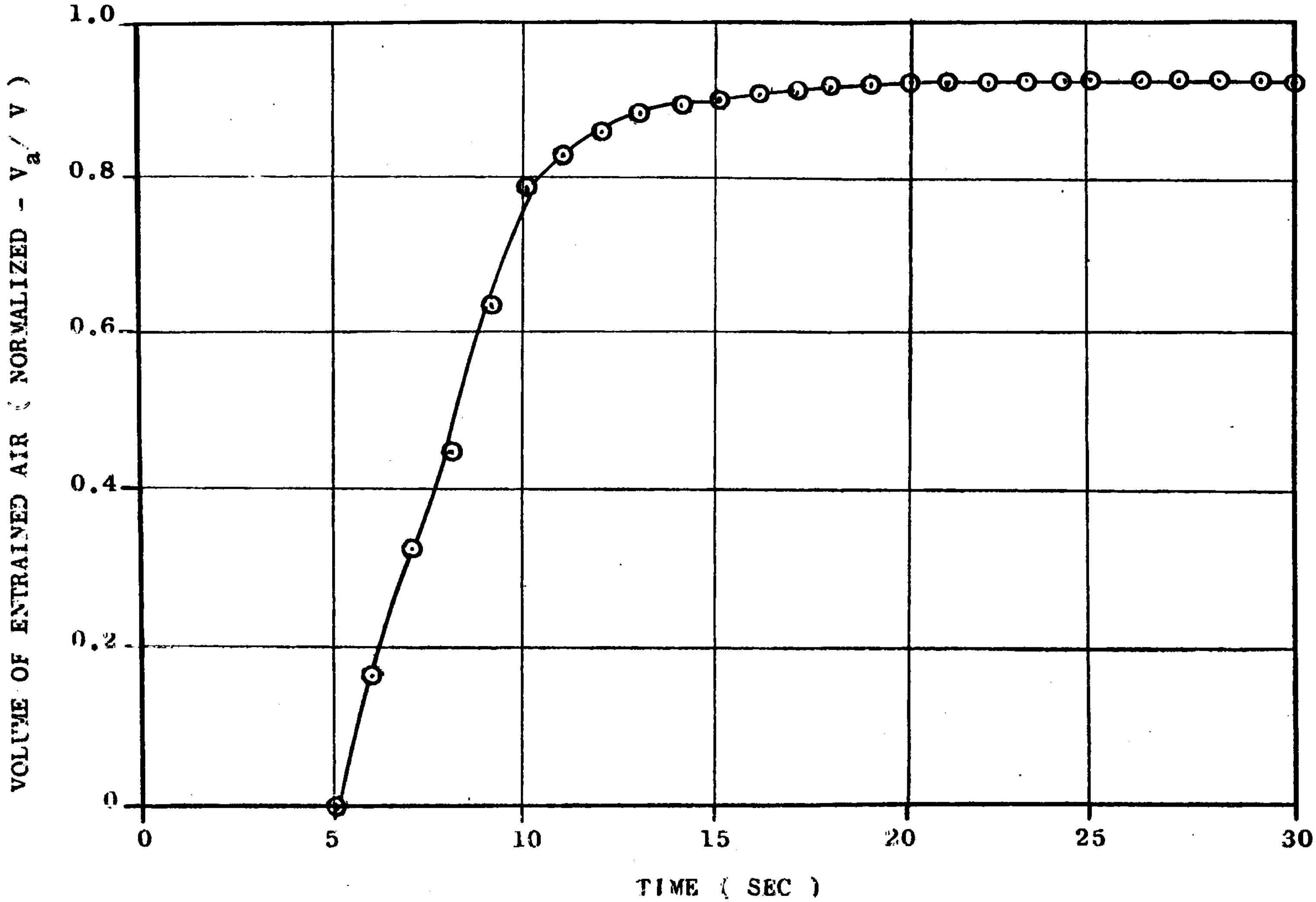


FIGURE 57-. VOLUME OF ENTRAINED AIR FOR RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

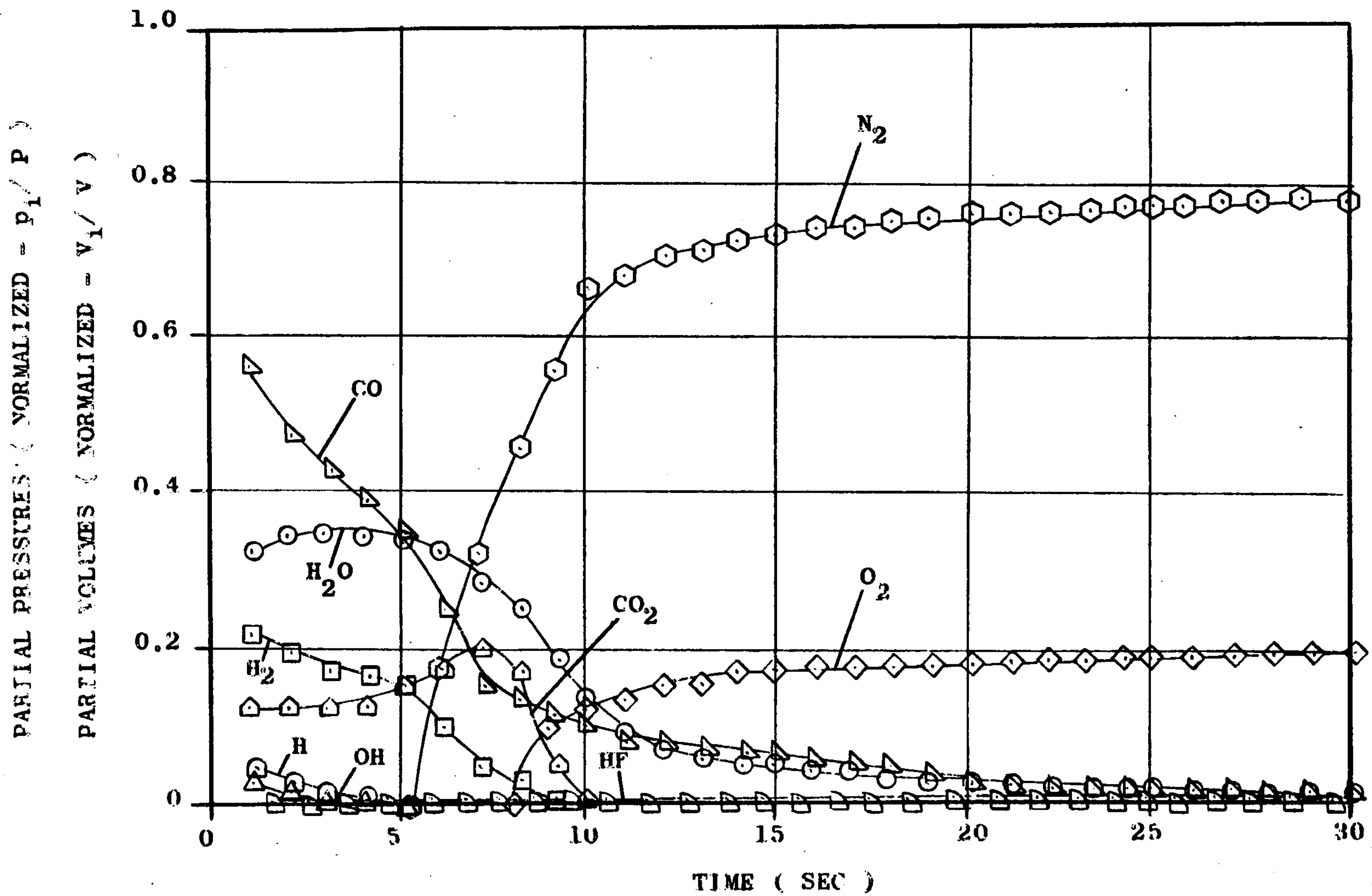


FIGURE 58. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

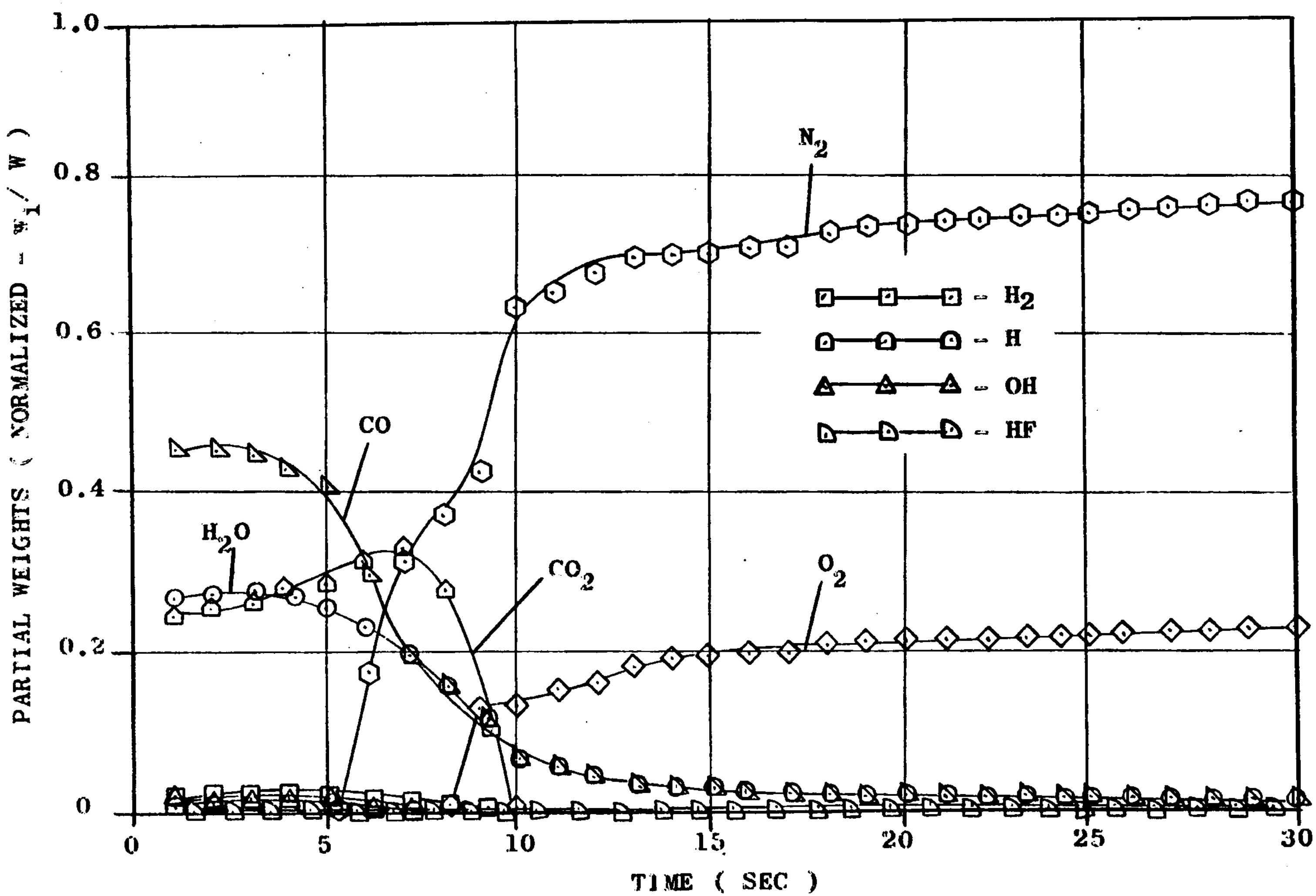


FIGURE 59-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM RP-1/LO_2+ 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

LH_2 / RP-1 / LO_2 + 1% F

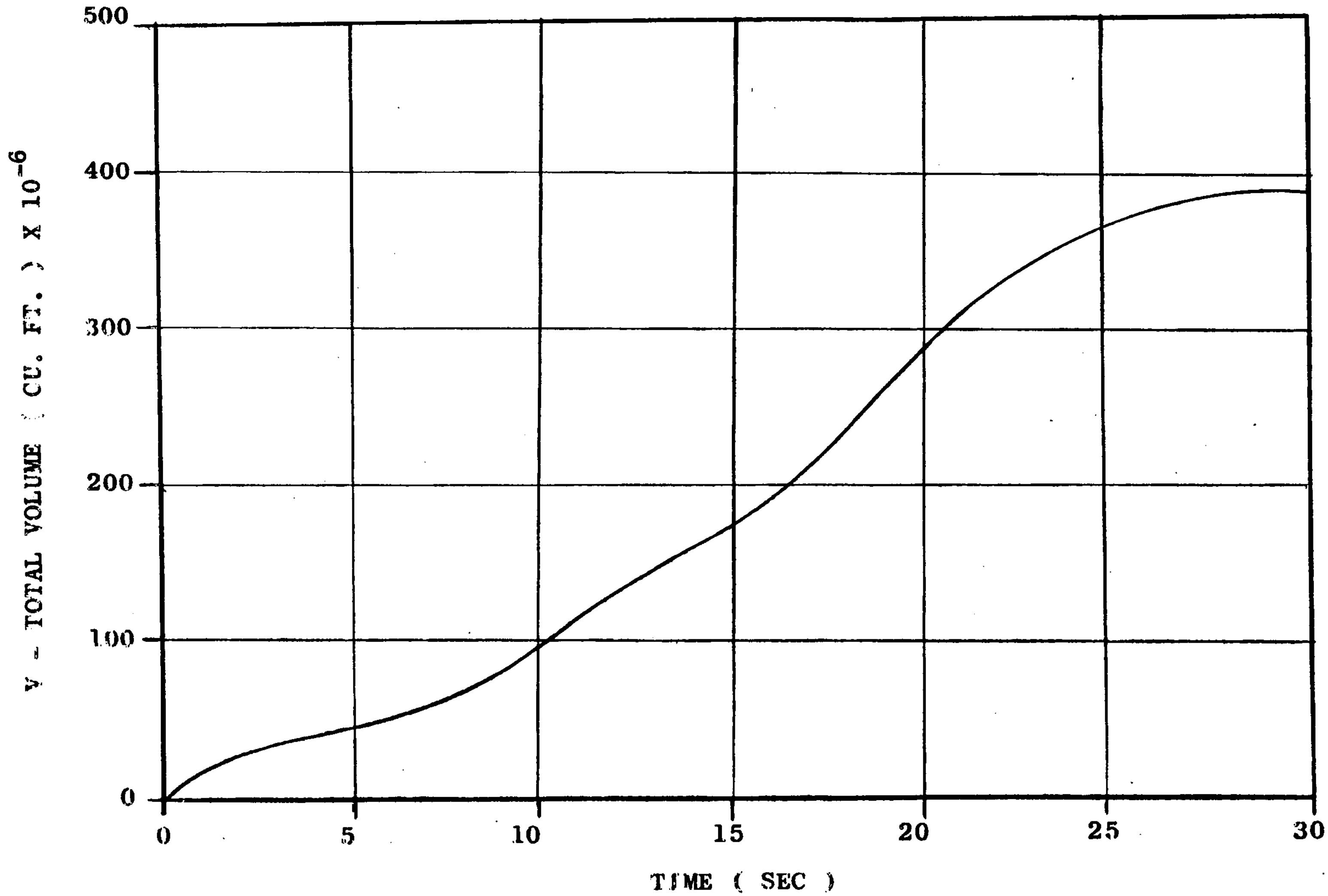


FIGURE 60-. VOLUME-TIME FUNCTION FOR $LH_2/RP\text{-}1/LO_2$ + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

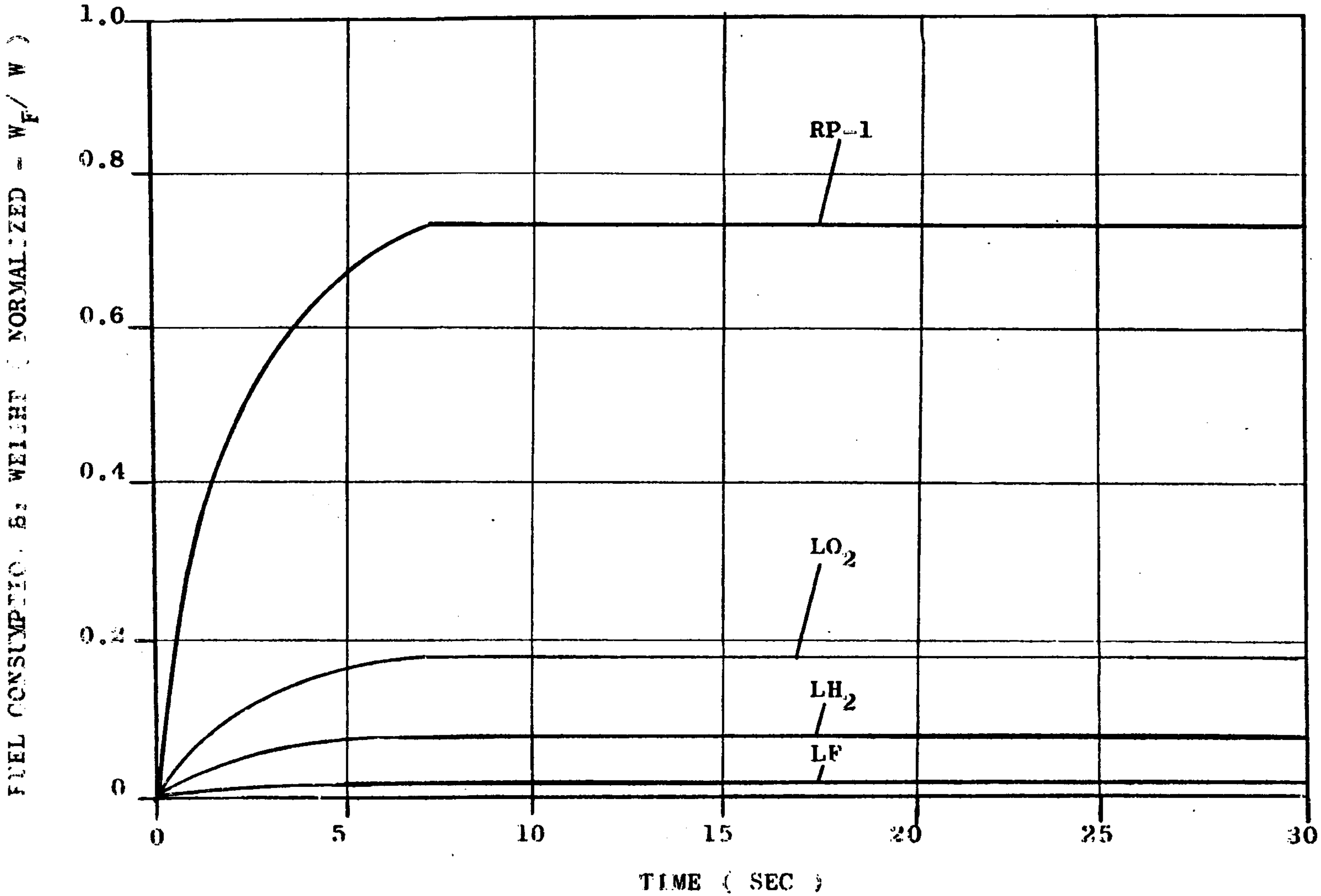


FIGURE 61-. FUEL CONSUMPTION FOR LH_2/RP-1/LO_2 + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

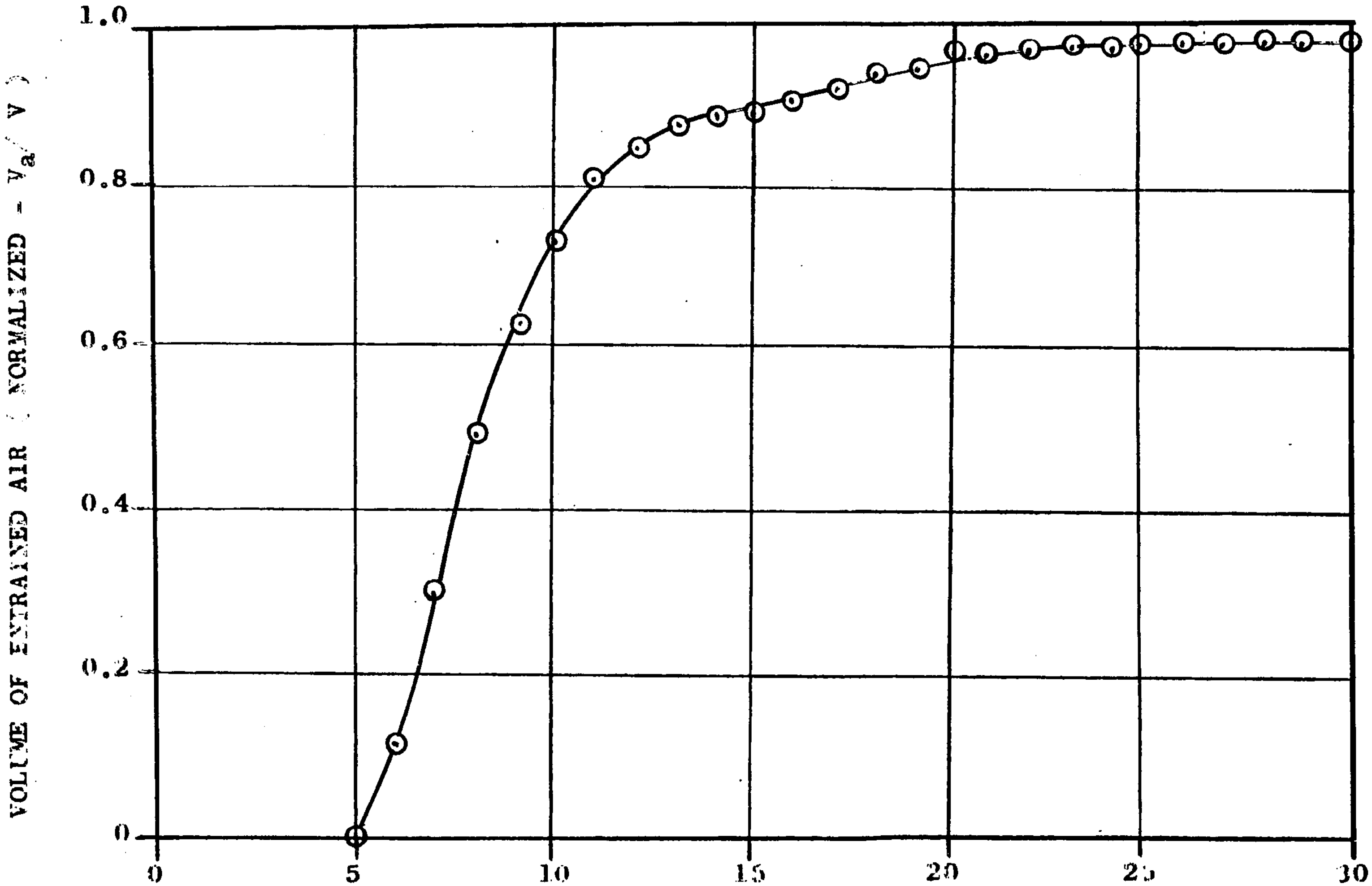


FIGURE 62-. VOLUME OF ENTRAINED AIR FOR $LH_2/RP\text{-}1/LO_2$ + 1% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

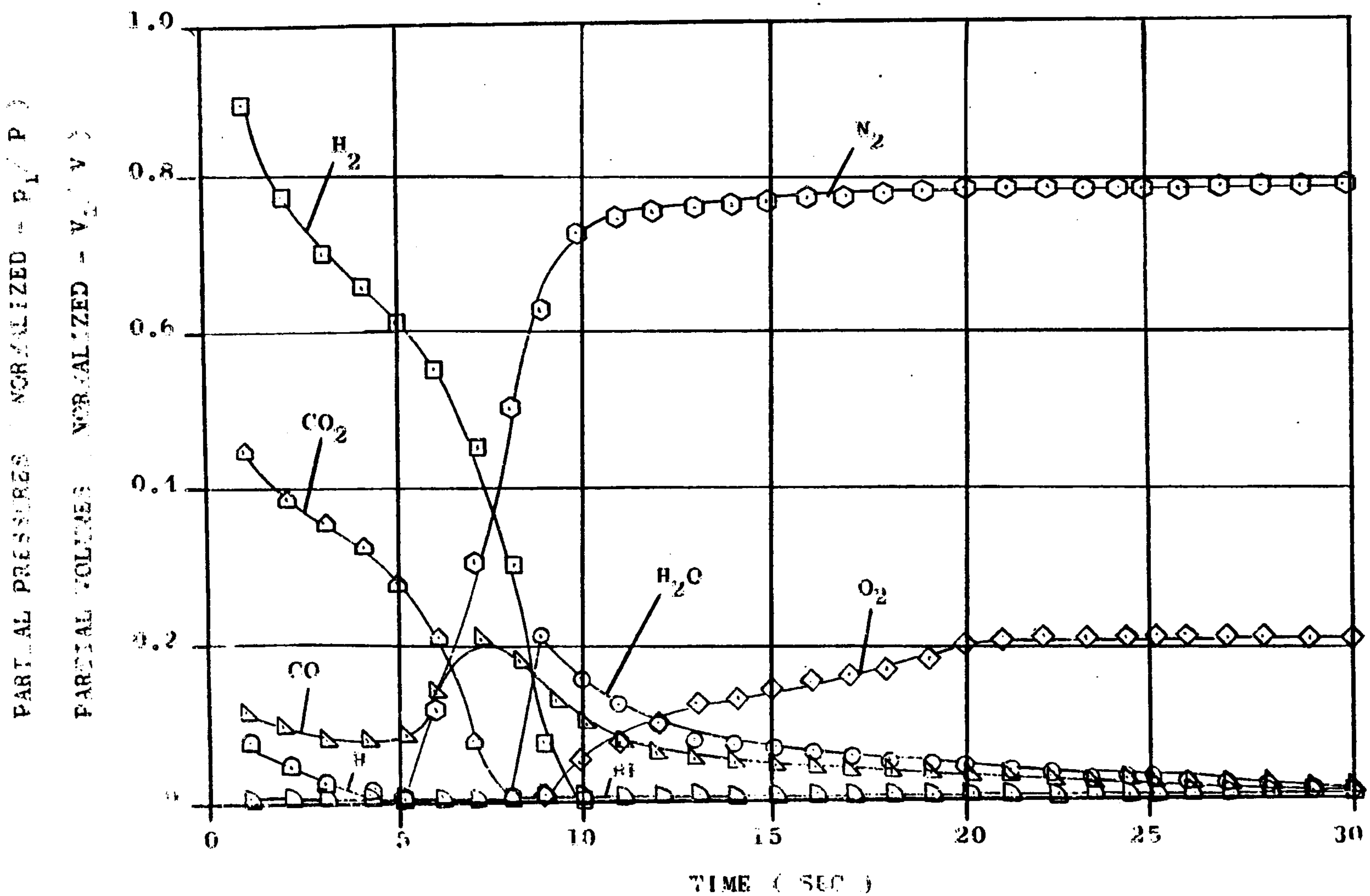


FIGURE 63-. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR $LH_2/RP\text{-}1/LO_2$ + 1% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

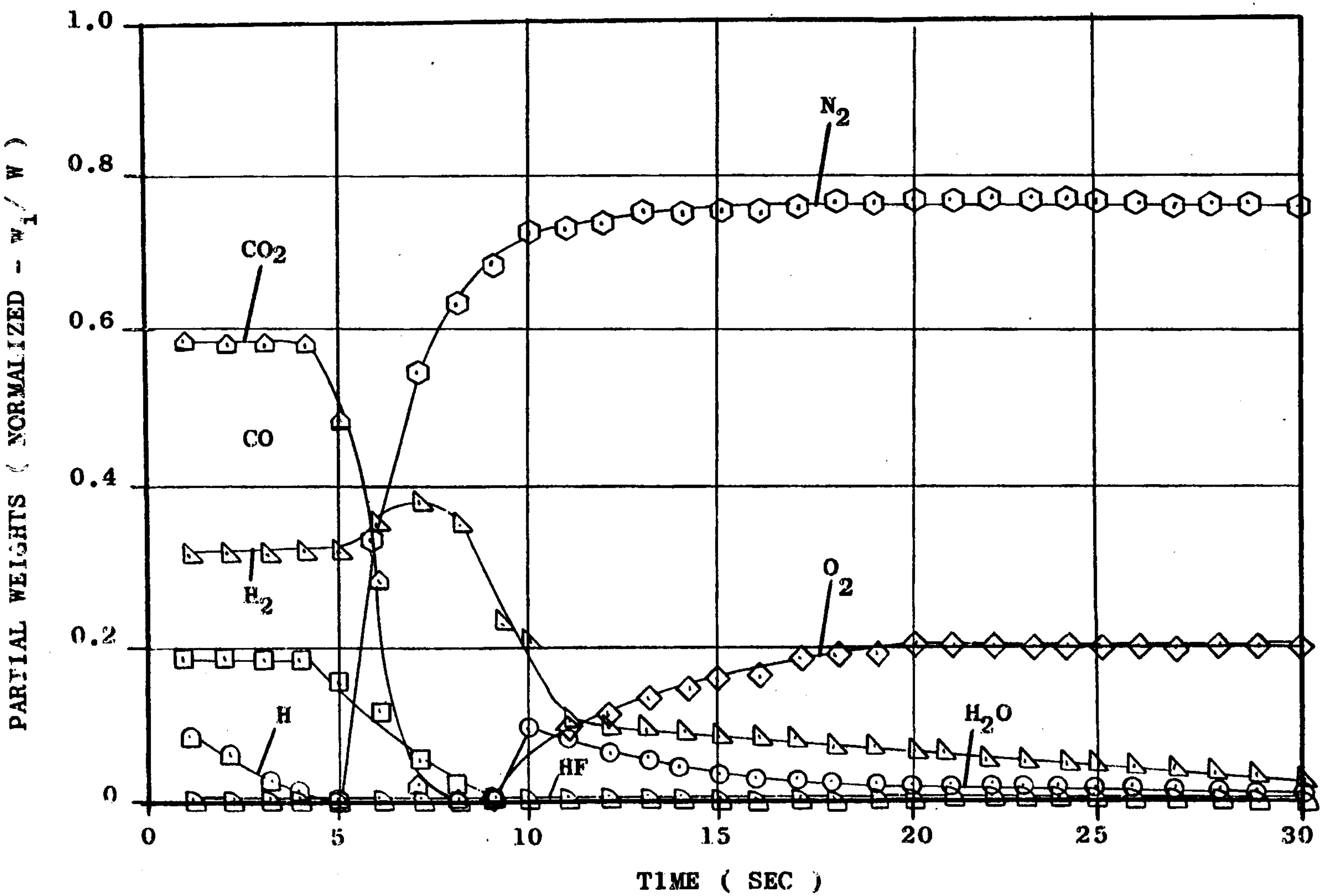


FIGURE 64-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/RP-1/LO_2+ 1% F LIQUID PROPELLANT EXPLOSION (YIELD ~ 4.5 PERCENT)

LH_2 / RP-1 / LO_2 + 5% F

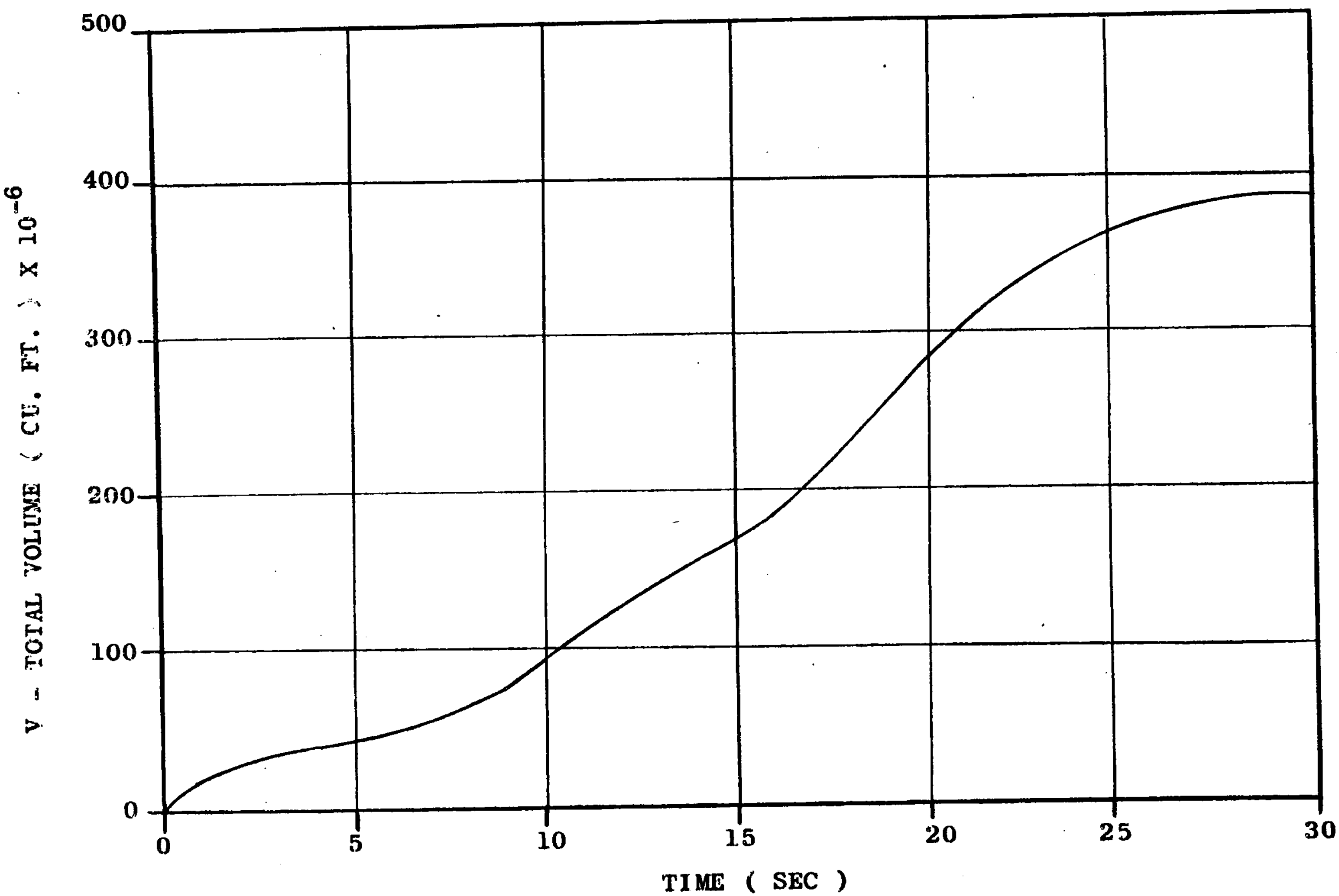


FIGURE 65-. VOLUME-TIME FUNCTION FOR $LH_2/RP\text{-}1/LO_2$ + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

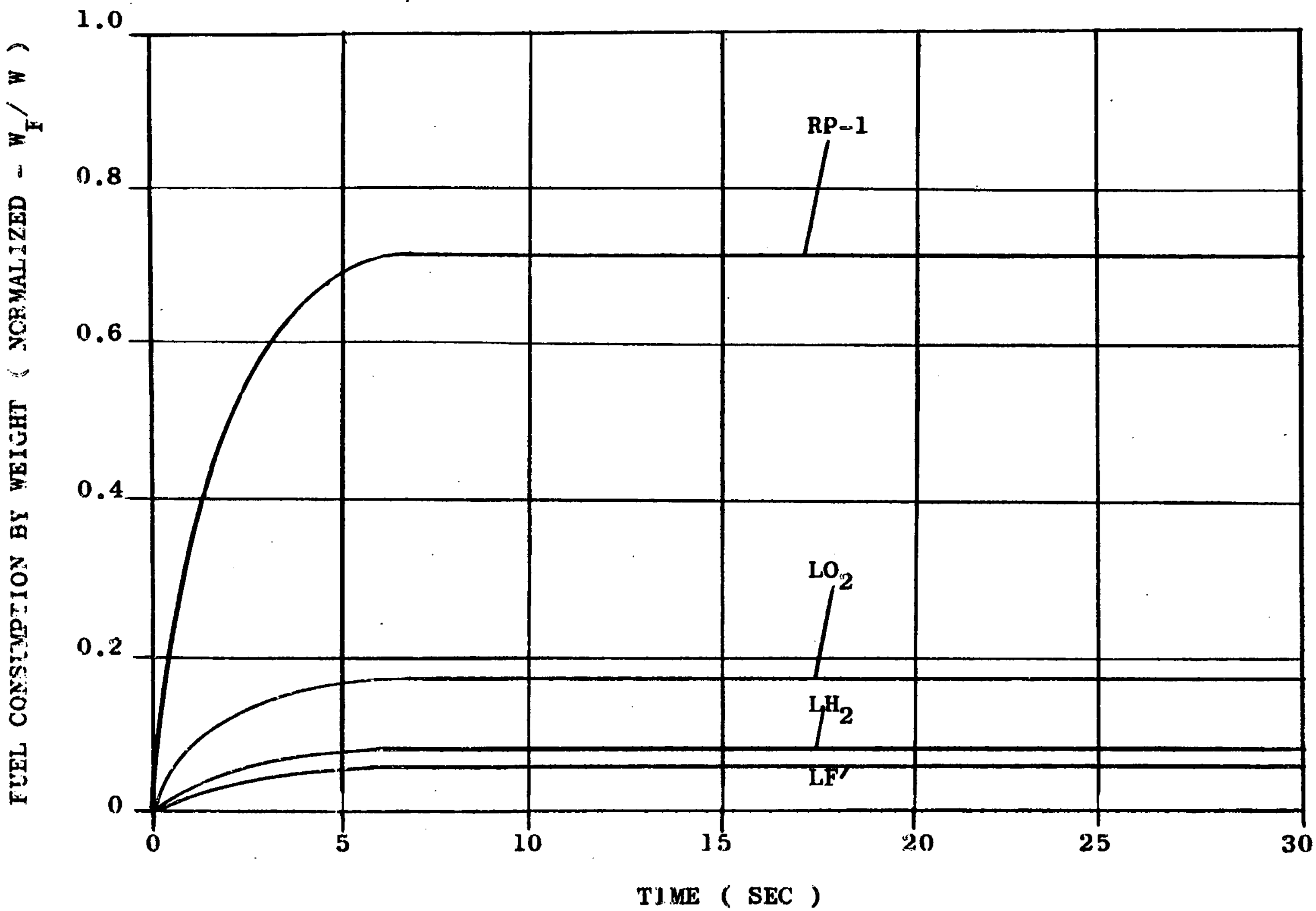


FIGURE 66-. FUEL CONSUMPTION FOR $LH_2/RP\text{-}1/LO_2$ + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

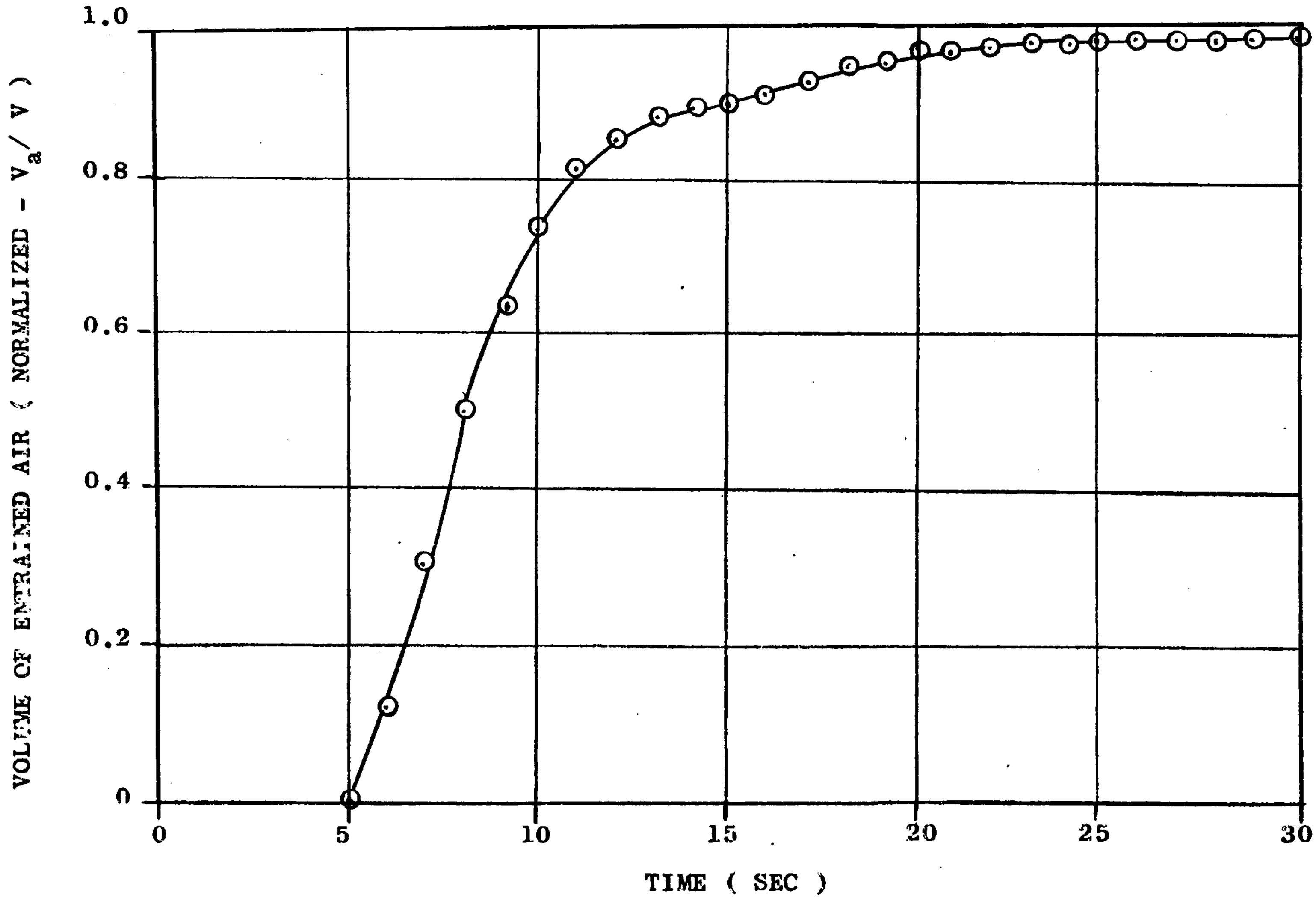


FIGURE 67-. VOLUME OF ENTRAINED AIR FOR LH_2/RP-1/LO_2 + 5% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

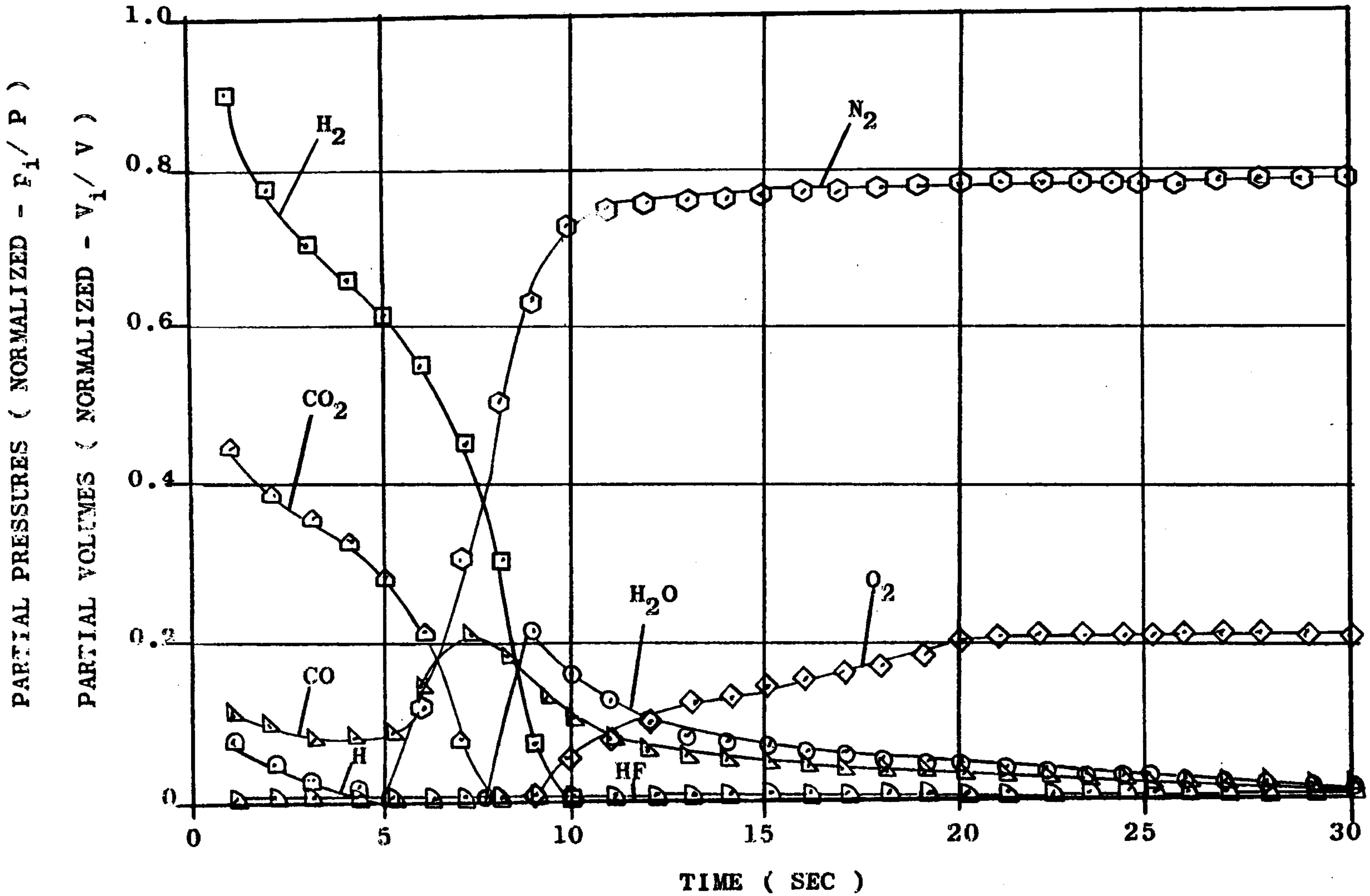


FIGURE 68--. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR $LH_2/RP\text{-}1/LO_2$ + 5% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

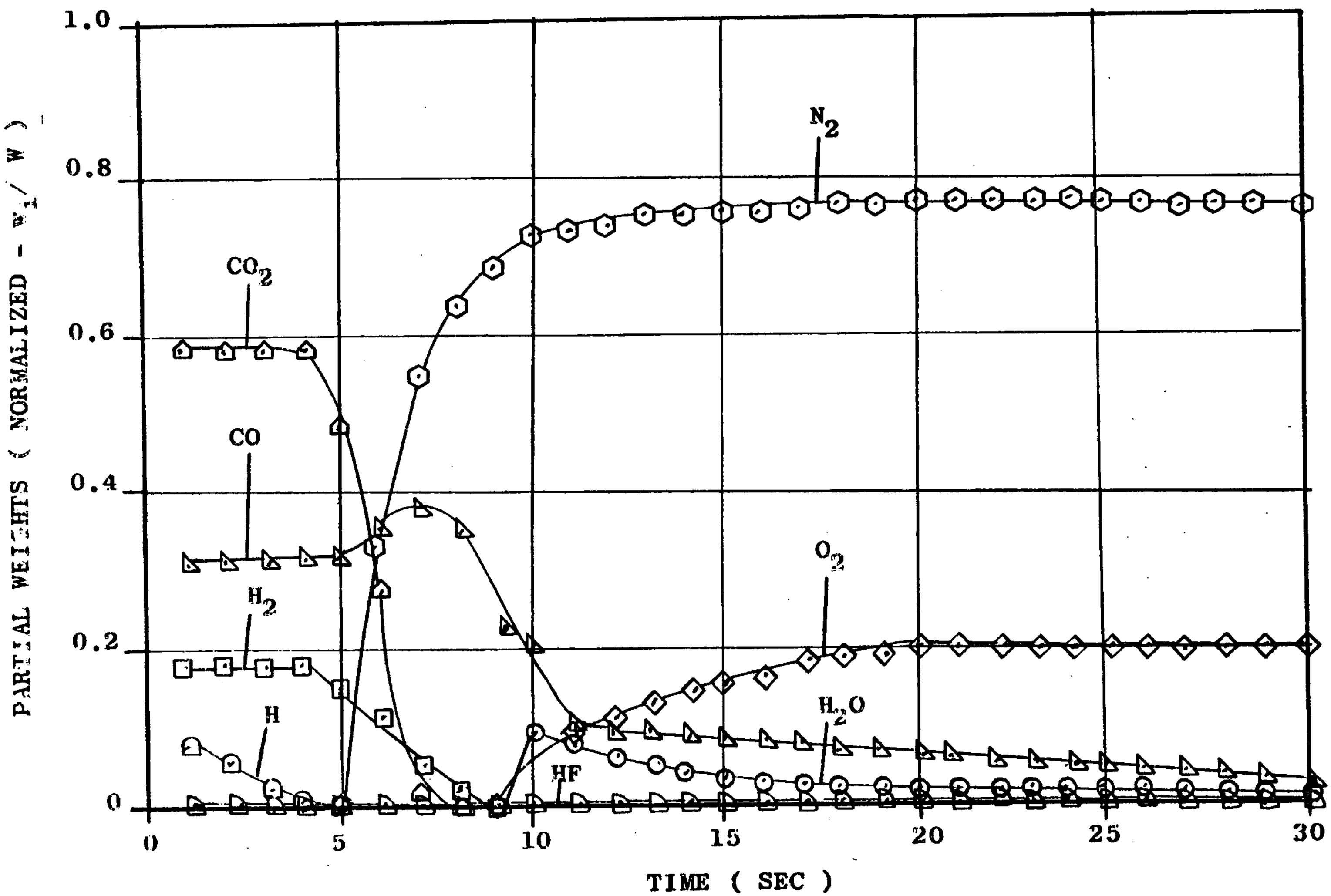


FIGURE 69-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/RP-1/LO_2+ 5%F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

LH_2 / RP-1 / LO_2 + 10% F

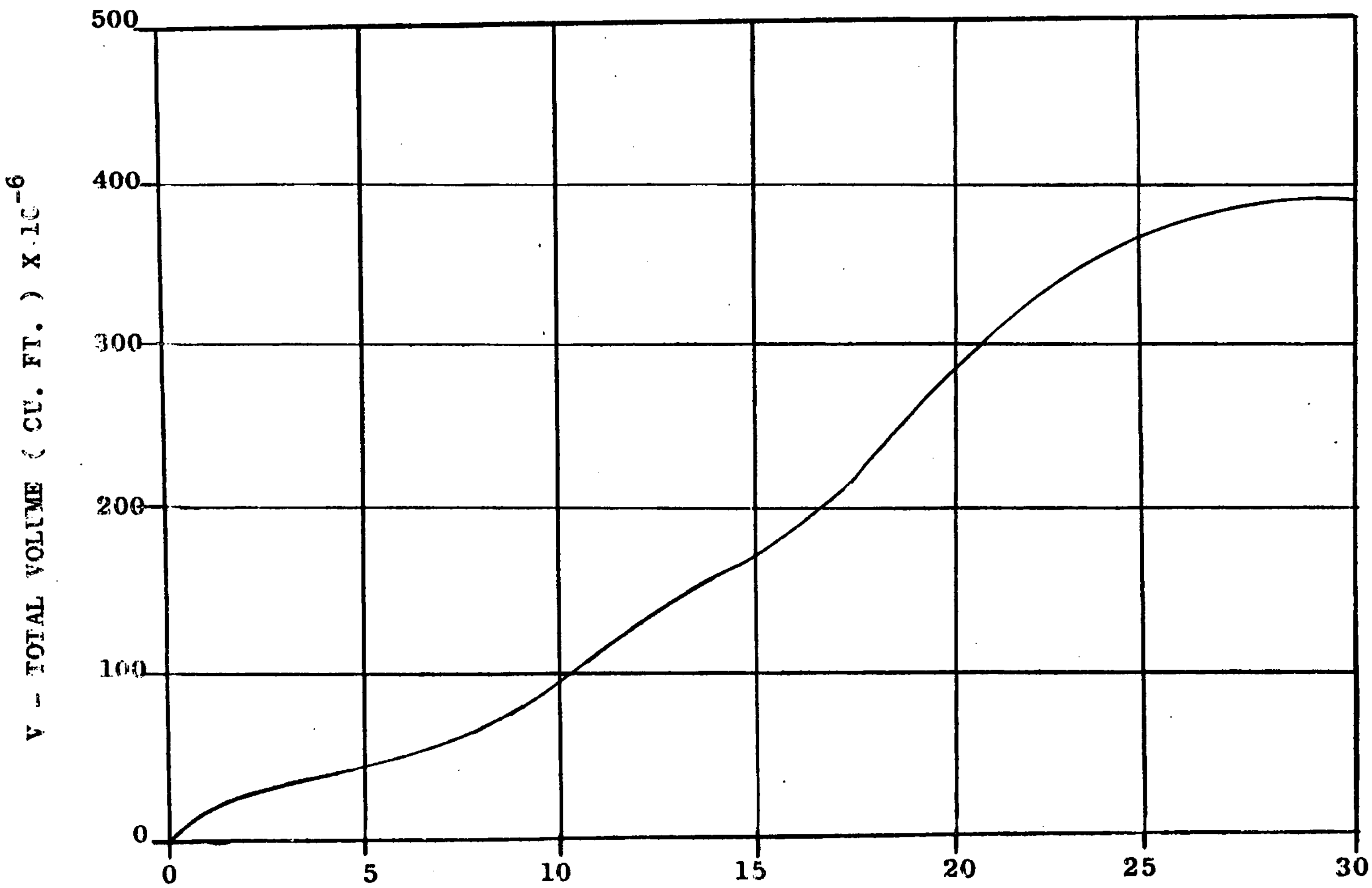


FIGURE 70-. VOLUME-TIME FUNCTION FOR $LH_2/RP\text{-}1/LO_2$ + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

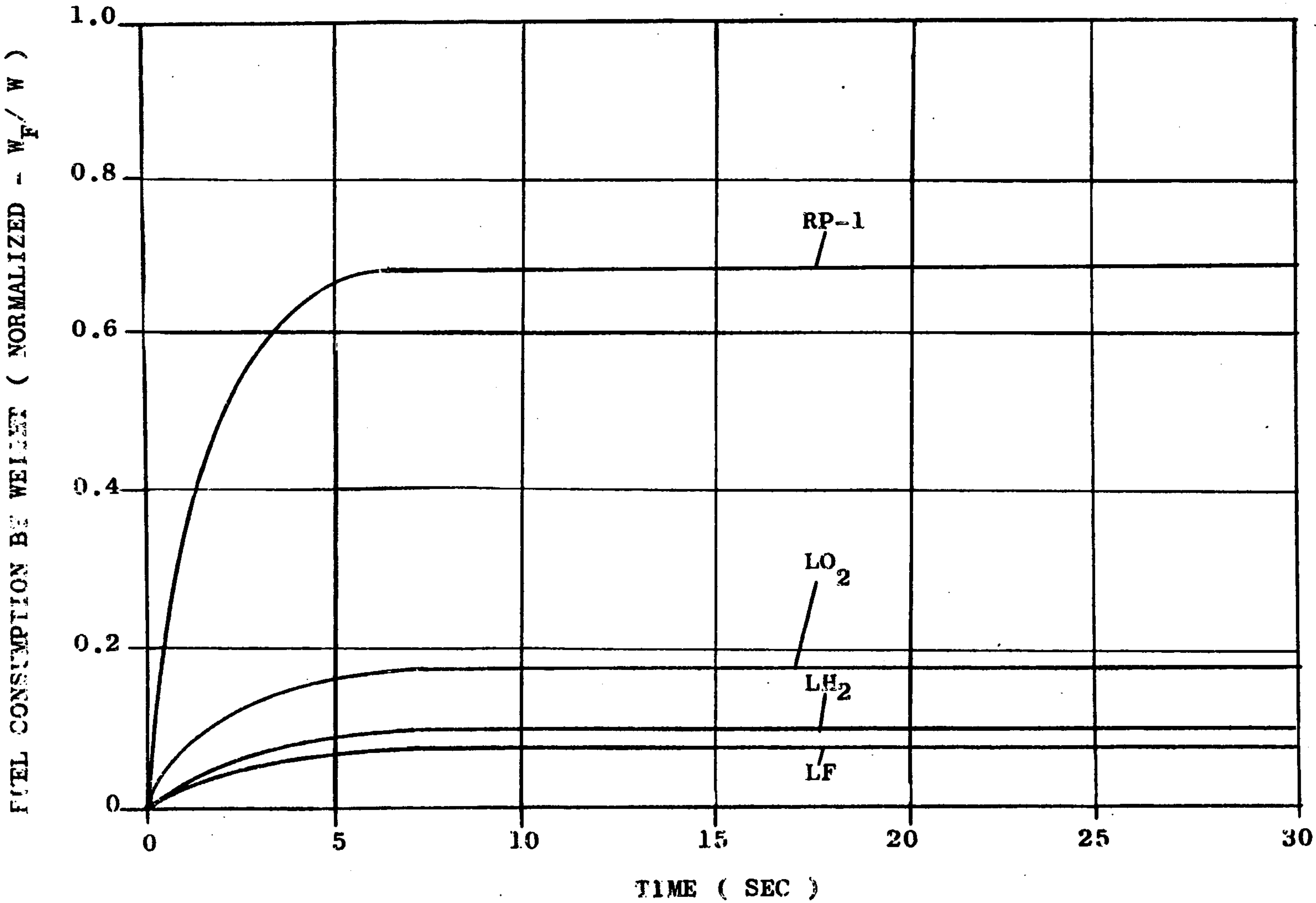


FIGURE 71-. FUEL CONSUMPTION FOR LH_2/RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

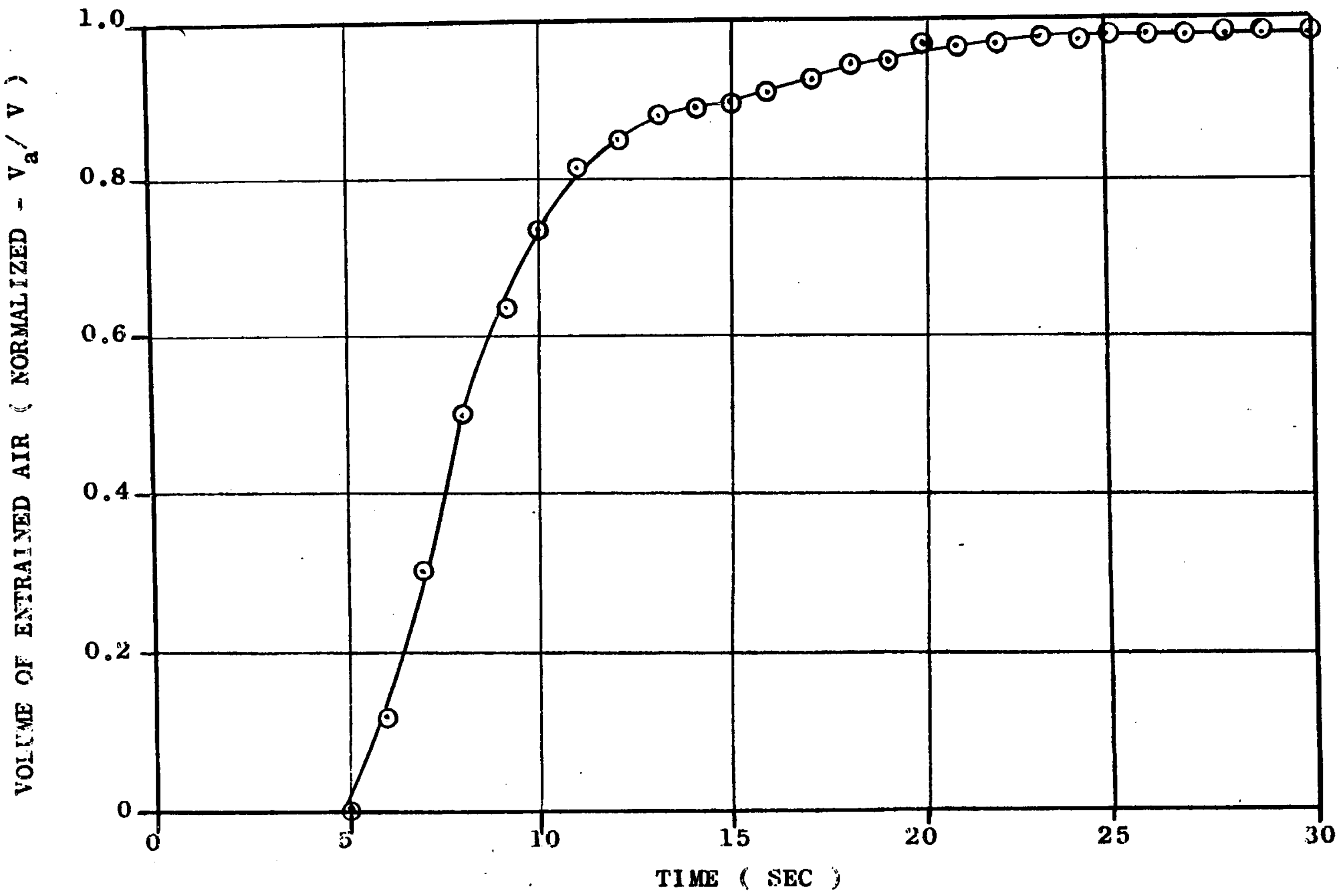


FIGURE 72. VOLUME OF ENTRAINED AIR FOR LH_2/RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

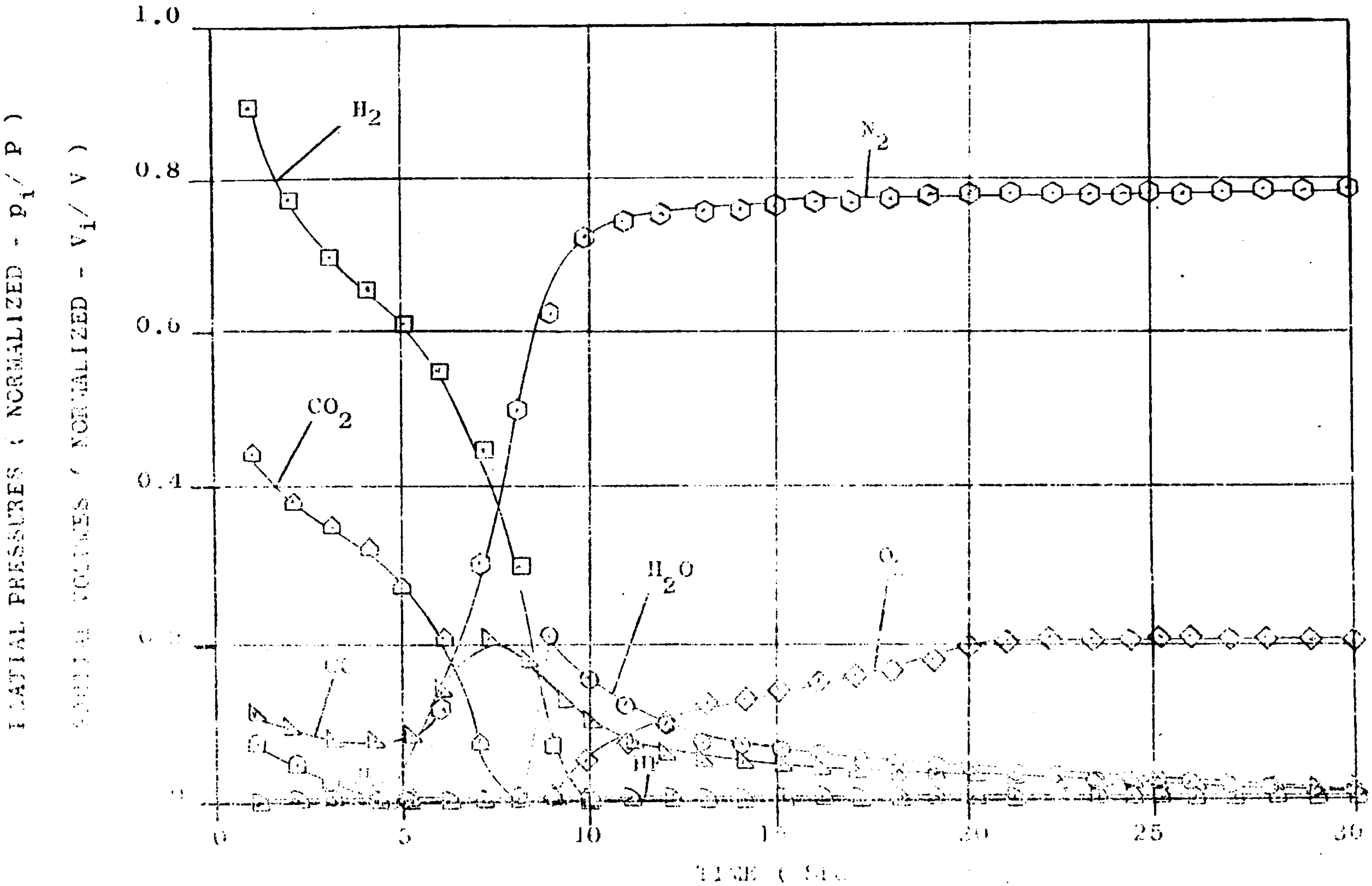


FIGURE 73. PARTIAL PRESSURES AND PARTIAL VOLUMES FOR LH_2/RP-1/LO_2 + 10% F LIQUID PROPELLANT EXPLOSION PRODUCTS (YIELD = 4.5 PERCENT)

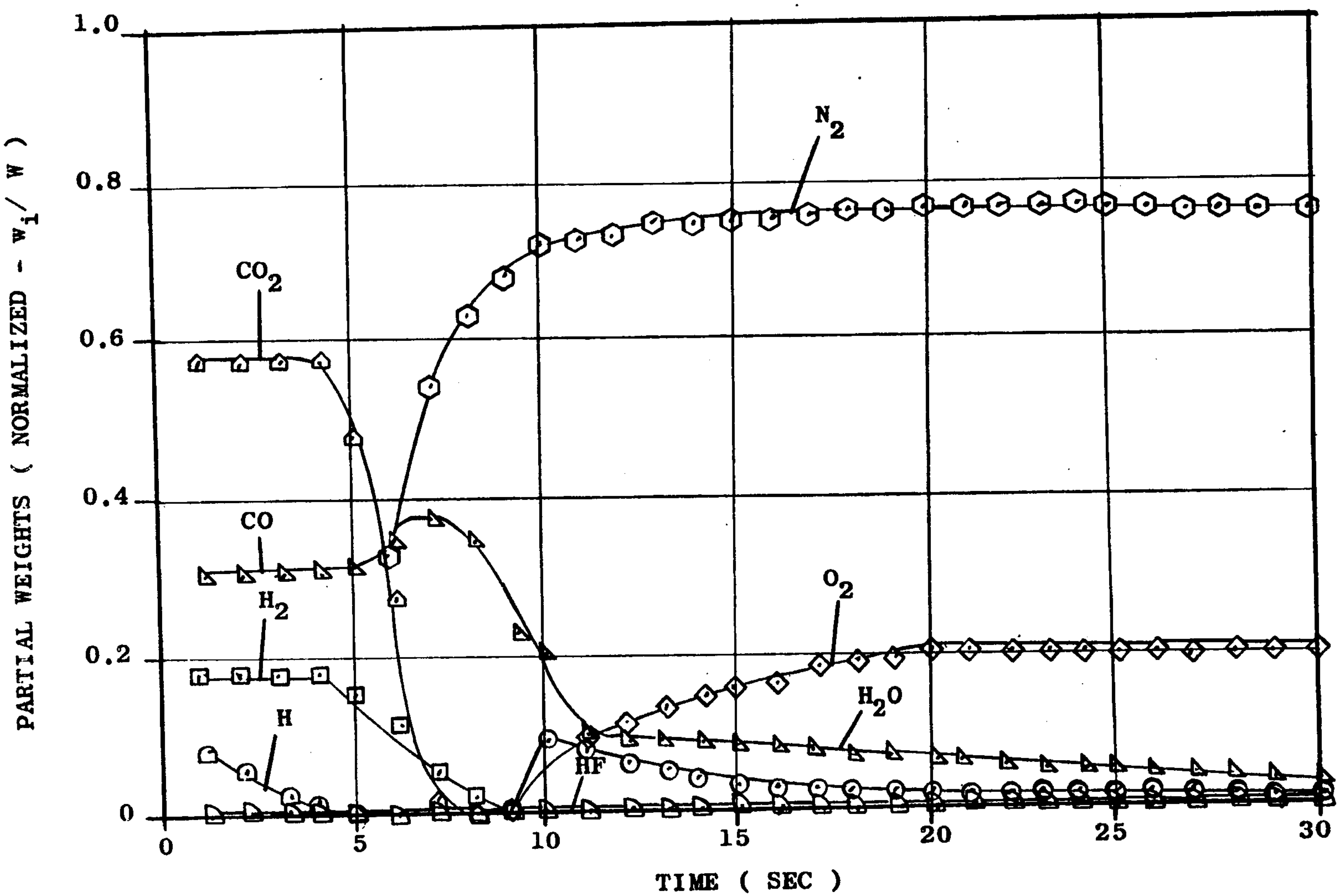


FIGURE 74-. WEIGHT COMPOSITION OF THE COMBUSTION PRODUCTS FROM LH_2/RP-1/LO_2+ 10%F LIQUID PROPELLANT EXPLOSION (YIELD = 4.5 PERCENT)

APPENDIX

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I Reaction Products

```
• 148218     STEWART              •060• REACTION PRODUCTS
$IBJOB         GL
$IBFTC MAIN     NODECK
      DIMENSION A(15,15),B(15),T(9),C(10,9),PT(15),P(15),PR(15),V(9)
      DIMENSION WT(15),WMOL(15),WTR(15),TNT(15)
      READ(5,102) X, MA
      READ(5,105) (T(J),J=1,9)
      READ(5,110)(PT(J),J=1,9)
      READ(5,106) ((C(I,J),J=1,9),I=1,10)
      READ (5,99) (WMOL(J), J=1,8)
      READ (5,99) (WMOL(J), J=9,15)
      DO 7 I=1,10
      DO 7 J=1,9
      IF(C(I,J)-88.03/2.3)31,32,32
   32 C(I,J)=88./2.31
   31 CONTINUE
    7 C(I,J)=10.**C(I,J)
      READ (5,100) YIELD
      DO 10 KLJ=1,MA
      READ (5,103) (V(J), J=1,5)
      READ (5,103) (V(J), J=6,9)
      READ (5,101) H2, RP1, O2, F2
      B1=H2/2.016
      B2 =RP1/(14.026*X)
      B3=O2/32.
      B4=F2/38.
      A1=YIELD*B1
      A2=YIELD*B2
      A3=YIELD*B3
      A4=YIELD*B4
      IF(A1)300,300,301
  300 A1=.01
  301 IF(A2)302,302,303
  302 A2=.01
  303 IF(A3)304,304,305
  304 A3=.01
  305 IF(A4)306,306,307
  306 A4=.01
  307 A5=.01
      DO 222 I=1,15
  222 P(I)=PT(1)/15.
      DO 10 J=1,9
      TNE=PT(J)*V(J)/(T(J)*1.314)
      WRITE (6,220)
      WRITE (6,130) H2
      WRITE (6,131) RP1
      WRITE (6,132) O2
      WRITE (6,133) F2
      WRITE (6,134)
      WRITE (6,135) T(J)
      WRITE (6,136) PT(J)
      WRITE (6,137) V(J)
      IF(J-1)600,600,601
  600 WRITE(6,237)YIELD
  601 WRITE (6,138)
      WRITE (6,139)
      WRITE (6,140)
      WRITE (6,141)
      WRITE (6,142)
      KL=0
    8 KL=KL+1
```

```
      Y1=2.*(A3+0.209*A5)
      Y2=2.*(A1+A2*X)
      Y3=1.584*A5
      Y4=A2*X
      Y5=2.*A4
      DO 1I=1,15
      DO 1K=1,15
    1 A(I,K)=0.0
      DO 2I=1,15
    2 A(I,I)=-1.0
      DO 3K=6,15
      I=K-5
    3 A(K,I)=1.0
      A(2,1)= 2.0*Y1-Y2
      A(2,2)= -2.0*Y2
      A(2,3)= 2.0*Y1
      A(2,6)= -2.0*Y2
      A(2,7)=Y1
      A(2,8)=-Y2
      A(2,9)=-Y2
      A(2,10)= Y1-Y2
      A(2,11)= Y1
      A(2,15)= -Y2
      A(3,1)= 2.0*Y3
      A(3,3)= 2.0*Y3
      A(3,4)= -2.0*Y2
      A(3,7)= Y3
      A(3,9)=-Y2
      A(3,10)= Y3
      A(3,11)= Y3
      A(3,12)= -Y2
      A(4,1)=2.*Y4
      A(4,2)=-Y2
      A(4,3)=2.*Y4
      A(4,7)=Y4
      A(4,8)=-Y2
      A(4,10)= Y4
      A(4,11)= Y4
      A(4,14)= -Y2
      A(5,1)=2.*Y5
      A(5,3)=2.*Y5
      A(5,5)=-2.*Y2
      A(5,7)=Y5-Y2
      A(5,10)= Y5
      A(5,11)= Y5
      A(5,13)= -Y2
      A(6,11)= -2.0*C(1,J)*P(11)*P(15)
      A(6,15)= -C(1,J)*P(11)**2
      A(7,14)= -C(2,J)*P(15)**2
      A(7,15)= -2.0*C(2,J)*P(14)*P(15)
      A(8,11)= -2.0*C(3,J)*P(11)
      A(9,12)= -2.0*C(4,J)*P(12)
      A(10,13)= -2.0*C(5,J)*P(13)
      A(11,15)= -2.0*C(6,J)*P(15)
      A(12,11) = -C(7,J)*P(13)
      A(12,13) = -C(7,J)*P(11)
      A(13,14) = -C(8,J)*P(15)
      A(13,15) = -C(8,J)*P(14)
      A(14,12) = -C(9,J)*P(15)
      A(14,15) = -C(9,J)*P(12)
      A(15,11)=-C(10,J)*P(15)
```

```
      A(15,15) = -C(10,J)*P(11)
      SUM = 0.
      DO 4I=1,15
    4 SUM=SUM+P(I)
      B(1)=PT(J)-SUM
      B(2)=(2.*Y1-Y2)*P(1)-2.*Y2*P(2)+2.*Y1*P(3)-2.*Y2*P(6)+Y1*P(7)
     1 -Y2*P(8)-Y2*P(9)+(Y1-Y2)*P(10)+Y1*P(11)-Y2*P(15)
      B(3)=2.*Y3*P(1)+2.*Y3*P(3)-2.*Y2*P(4)+Y3*P(7)-Y2*P(9)+Y3*P(10)+
     1Y3*P(11)-Y2*P(12)
      B(4)=2.*Y4*P(1)-Y2*P(2)+2.*Y4*P(3)+Y4*P(7)-Y2*P(8)+Y4*P(10)+Y4
     1 *P(11)-Y2*P(14)
      B(5)=2.*Y5*P(1)+2.*Y5*P(3)-2.*Y2*P(5)+(Y5-Y2)*P(7)+Y5*P(10)+Y5*P(1
     11)-Y2*P(13)
      B(6)=P(1)-C(1,J)*P(11)**2*P(15)
      B(7)=P(2)-C(2,J)*P(14)*P(15)**2
      B(8)=P(3)-C(3,J)*P(11)**2
      B(9)=P(4)-C(4,J)*P(12)**2
      B(10)=P(5)-C(5,J)*P(13)**2
      B(11)=P(6)-C(6,J)*P(15)**2
      B(12)=P(7)-C(7,J)*P(11)*P(13)
      B(13)=P(8)-C(8,J)*P(14)*P(15)
      B(14)=P(9)-C(9,J)*P(12)*P(15)
      B(15)=P(10)-C(10,J)*P(11)*P(15)
      DO 55I=1,15
   55 B(I)=-B(I)
      CALL INVERT(A,15,15,B,1,15,DETERM,IERROR)
      DO 6 I=1,15
      P(I)=P(I)+B(I)
      IF(P(I)) 41,6,6
   41 P(I)=0.0
    6 CONTINUE
      SUM1=0.
      DO 30 I= 1,15
   30 SUM1=SUM1+ABS(B(I))
      IF(SUM1-.0005)51,51,6
   51 TN=PT(J)*Y2/(2.*P(1)+2.*P(3)+P(7)+P(10)+P(11))
      TNR=TNE/TN
      IF(KL-150)25,25,50
   25 IF(V(J))50,50,49
   49 IF(ABS(TNR-1.)-.001)50,50,27
   27 IF(A1-0.01) 52,52,53
   53 A1=A1*TNR
      IF(B1-A1) 70,70,52
   70  A1= B1
   52 IF(A2-0.01) 54,54,95
   95 A2=A2*TNR
      IF(B2-A2)71,71,54
   71 A2=B2
   54 IF(A3-0.01) 56,56,57
   57 A3=A3*TNR
      IF (B3-A3) 72,72,56
   72 A3=B3
   56 IF( A4-0.01) 58,58,59
   59 A4=A4*TNR
      IF (B4-A4) 73,73,58
   73 A4=B4
   58 IF (B1-A1) 75,75,79
   75 IF(B2-A2 ) 76,76,79
   76 IF (B3-A3) 77,77,79
   77 IF(B4-A4) 78,78,79
   78 IF(A5-.01)80,80,68
```

```
   80 A5=TNE-TN
      GO TO 79
   88 A5=A5*TNR
   79 CONTINUE
   74 GO TO 8
   50 WRITE(6,104) KL
      WRITE(6,111)
      WRITE(6,112) (P(I), I=1,5)
      WRITE(6,112) (P(I), I=6,10)
      WRITE(6,112) (P(I), I=11,15)
      DO 214 I=1,15
      PR(I)=P(I)/PT(J)
      TNT(I)=PR(I)*TN
  214 WT(I)=TNT(I)*WMUL(I)
      WRITE(6,113)
      WRITE( 6,114) (TNT(I), I=1,5)
      WRITE (6,114) (TNT(I), I=6,10)
      WRITE (6,114) (TNT(I), I=11,15)
      WRITE(6,115)
      WRITE(6,112) (PR(I), I=1,5)
      WRITE(6,112) (PR(I), I=6,10)
      WRITE(6,112) (PR(I), I=11,15)
      WPROD=0.0
      DO 117 I=1,15
  117  WPROD=WPROD+WT(I)
      DO 118 I=1,15
  118 WTR(I)=WT(I)/WPROD
      WRITE(6,116)
      WRITE(6,119) (WT(I), I=1,5)
      WRITE (6,119)(WT(I), I=6,10)
      WRITE(6,119) (WT(I), I=11,15)
      WRITE(6,120)
      WRITE(6,212) ( WTR(I), I=1,5)
      WRITE (6,212) (WTR(I), I=6,10)
      WRITE (6,212) (WTR(I), I=11,15)
      WRITE(6,121)
      C1=A1*2.016
       C2=A2*(14.026*X)
      C3=A3*32.
      C4=A4*38.
      WRITE(6,122) C1
      WRITE(6,123) C2
      WRITE (6,124) C3
      WRITE(6,125) C4
      WRITE( 6,126)
      WRITE(6,127) A5
      WAIR=A5*28.966
      WRITE(6,128) WAIR
      RNAIR=A5/TN
      RWAIR=WAIR/WPROD
      WRITE(6,129) RNAIR
      WRITE(6,230) RWAIR
      WRITE(6,161) TN
      TVOL=TN*T(J)*1.314/PT(J)
      WRITE(6,143) TVOL
   10 CONTINUE
  102 FORMAT(F5.1,I3)
  105 FORMAT(9F6.0)
  110 FORMAT(9F6.2)
  106 FORMAT(9F8.4)
  103 FORMAT(5F12.0)
```

```
  99 FORMAT(8F7.3)
 100 FORMAT( F7.4)
 101 FORMAT(4F10.2)
 220 FORMAT(/////,8X,28HAMOUNT OF PROPELLANT,POUNDS   )
 130 FORMAT(12X,4HLH2=F10.2)
 131 FORMAT(12X,5HRP-1=F10.2)
 132 FORMAT(12X,4HLO2=F10.2)
 133 FORMAT(12X,4HLF2=F10.2)
 134 FORMAT(//,6X,34HEXPERIMENTAL VALUES OF T,P,V        )
 135 FORMAT(/,12X,16HDEGREES KELVIN =F7.1)
 136 FORMAT(12X,12HATMOSPHERES=F6.1)
 137 FORMAT(12X,11HCUBIC FEET=F12.0)
 237 FORMAT(12X,6HYIELD=F7.4)
 138 FORMAT(//,13X,20HTHEORETICAL RESULTS )
 139 FORMAT(/,8X,39HIDENTIFICATION OF PRODUCTS OF REACTION )
 140 FORMAT(/,8X,3HH2C,5X,3HCO2,5X,2HH2,6X,2HN2,6X,2HF2)
 141 FORMAT(8X,2HO2,6X,2HHF,6X,2HCO,6X,2HNO,6X,2HOH)
 142 FORMAT(8X,1HH,7X,1HN,7X,1HF,7X,1HC,7X,1HO)
 104 FORMAT(8X,I3,20H ITERATIONS REQUIRED)
 111 FORMAT(/,19X,17HPARTIAL PRESSURES)
 112 FORMAT(8X,5(F7.3,1X))
 113 FORMAT(/,32X,11HPOUND MOLES)
 114 FORMAT(5X,5(F12.2,1X))
 115 FORMAT(/,14X,27HPRESSURE,MOLE,VOLUME RATIOS )
 116 FORMAT(/,32X,13HPOUND WEIGHTS)
 119 FORMAT(5X,5( F12.0,1X))
 120 FORMAT(/,19X,13HWEIGHT RATIOS)
 212 FORMAT(8X,5F7.4)
 121 FORMAT(/,8X,19HBURNING RATE,POUNDS)
 122 FORMAT(9X,4HLH2=F12.0)
 123 FORMAT(9X,5HRP-1=F12.0)
 124 FORMAT(9X,4HLO2=F12.0)
 125 FORMAT(9X,4HLF2=F12.0)
 126 FORMAT(/,8X,23HAMOUNT OF ENTRAINED AIR)
 127 FORMAT(8X,6HMOLES=F12.0)
 128 FORMAT(8X,7HPOUNDS=F12.0)
 129 FORMAT(8X,27HPRESSURE,MOLE,VOLUME RATIO=F8.3)
 230 FORMAT(8X,13HWEIGHT RATIO=F7.4)
 161 FORMAT(/,8X,30HTOTAL THEORETICAL POUND MOLES=F12.0)
 143 FORMAT(/,8X,19HTHEORETICAL VOLUME=F12.0)
     RETURN
     END
$DATA
 11.6  3
 3000. 2800. 2600. 2400. 2200. 2000. 1800. 1600. 1400.
 31.7   1.52  1.25  1.12  1.05  1.     1.     1.     1.
  3.8617  5.0661  6.4532  8.0683  9.9730 12.2533 15.0332 18.4983 22.9395
 13.0585 15.0772 17.4062 20.1232 23.3337 27.1655 31.8923 37.7738 45.3324
  1.6064  2.1772  2.8344  3.5994  4.5010  5.5798  6.8941  8.5311 10.6275
  5.7261  6.6404  7.6940  8.9216 10.3703 12.1063 14.2247 16.8684 20.2614
 -3.9111 -3.7015 -3.4608 -3.1816 -2.8534 -2.4618 -1.9659 -1.3945  -.6388
  1.8415  2.4756  3.2066  4.0586  5.0643  6.2695  7.7403  9.5756 11.9307
  3.6997  4.4307  5.2726  6.2528  7.4086  8.7922 10.4788 12.5810 15.2752
 11.6713 13.0338 14.6045 16.4352 18.5966 21.1878 24.3515 28.3020 33.3754
  2.8677  3.5299  4.2927  5.1811  6.2293  7.4846  9.0165 10.9274 13.3789
  1.7434  2.2979  2.9363  3.6792  4.5549  5.6027  6.8793  8.4697 10.5067
 18.016 44.01   2.016 28.016 38.     32.     20.008 28.01
 30.008 17.008  1.008 14.008 19.     12.01   16.
  .045
          0.    12000000.    17500000.    20000000.    2100000.
   21000000.    25500000.    34000000.    44500000.
```

```
16700.00       0.00  83300.00    5000.00
      0.     6500000.     9500000.    11300000.    12000000.
 13000000.   15000000.   18500000.    23000000.
   0.00  30800.00  69200.00    5000.00
      0.    21000000.    29000000.    34500000.    38000000.
 40000000.   47000000.   60000000.    76000000.
 7000.00  75300.00  17700.00    5000.00
```

NDFILE

II Subroutine Invert

```
      SUBROUTINE INVERT (A,NA1,NAD1,B,NB1,NBD1,DETERM,IERROR)
      DIMENSION INDEX(100) , B1(100) , A(1) , B(1)                      609
      EQUIVALENCE (B1,INDEX)                                            609
C                INITIALIZE                                             609
    1 CALL OVERFL (INDEX)                                               609
   10 NA = NA1                                                          609
      NAD = NAD1                                                        609
      NB = NB1                                                          609
      NBD = NBD1                                                        609
      DET = 1.0                                                         609
      IERROR = 0                                                        609
      DO 20 I = 1,NA                                                    609
   20 INDEX(I) = -1                                                     609
      DO 130 I = 1,NA                                                   609
C                SEARCH FOR PIVOTAL ELEMENT                             609
      PIVOT = 0.0                                                       609
      IJ =  0                                                           609
      DO 60 J = 1,NA                                                    609
      IF(INDEX(J)) 30,250,60                                            609
   30 DO 55 II = 1,NA                                                   609
      IF(INDEX(II)) 40,250,55                                           609
   40 IJ1 = IJ + II                                                     609
      IF(ABS (PIVOT) - ABS (A(IJ1))) 50,55,55                           609
   50 IROW = II                                                         609
      JCOL = J                                                          609
      PIVOT = A(IJ1)                                                    609
   55 CONTINUE                                                          609
   60 IJ = IJ + NAD                                                     609
      IF(PIVOT) 65,250,65                                               609
   65 INDEX(JCOL) =IABS (INDEX(JCOL))                                   609
C                INTERCHANGE ROWS TO PUT PIVOTAL ELEMENT ON DIAGONAL    609
      IF(IROW - JCOL) 70,90,70                                          609
   70 DET = -DET                                                        609
      IJ = IROW                                                         609
      IJ1 = JCOL                                                        609
      DO 80 J = 1,NA                                                    609
      SAVE = A(IJ)                                                      609
      A(IJ) = A(IJ1)                                                    609
      A(IJ1) = SAVE                                                     609
      IJ = IJ + NAD                                                     609
   80 IJ1 = IJ1 + NAD                                                   609
   90 INDEX(I) = INDEX(I) * (1000 * IROW + JCOL)                        609
      DET = DET * PIVOT                                                 609
C                DIVIDE PIVOTAL ROW BY PIVOTAL ELEMENT                  609
      IJ = JCOL + (JCOL - 1) * NAD                                      609
      A(IJ) = 1.0                                                       609
      IJ = JCOL                                                         609
      DO 100 J = 1,NA                                                   609
      A(IJ) = A(IJ) / PIVOT                                             609
  100 IJ = IJ + NAD                                                     609
C                REDUCE NON-PIVOTAL ROWS                                609
      IJ = (JCOL - 1) * NAD                                             609
      DO 130 II = 1,NA                                                  609
      IJ = IJ + 1                                                       609
      IF(II - JCOL) 110,130,110                                         609
  110 SAVE = A(IJ)                                                      609
      A(IJ) = 0.0                                                       609
      IJ2 = JCOL                                                        609
      IJ1 = II                                                          609
      DO 120 J = 1,NA                                                   609
      A(IJ1) = A(IJ1) - A(IJ2) * SAVE                                   609
```

```
      IJ1 = IJ1 + NAD                                                   609
  120 IJ2 = IJ2 + NAD                                                   609
  130 CONTINUE                                                          609
      DETERM = DET                                                      609
C                 INTERCHANGE COLUMNS                                   609
      DO 160 K = 1,NA                                                   609
      J = NA + 1 - K                                                    609
      IROW = INDEX(J) / 1000                                            609
      JCOL = INDEX(J) - IROW * 1000                                     609
      IF(JCOL - IROW) 140,160,140                                       609
  140 IJ = (IROW - 1) *NAD                                              609
      IJ1 = (JCOL - 1) *NAD                                             609
      DO 150 I = 1,NA                                                   609
      IJ = IJ + 1                                                       609
      IJ1 = IJ1 + 1                                                     609
      SAVE = A(IJ)                                                      609
      A(IJ) = A(IJ1)                                                    609
  150 A(IJ1) = SAVE                                                     609
  160 CONTINUE                                                          609
C                 A INVERSE IS NOW STORED IN A                          609
C                 FIND SOLUTION VECTORS FOR ALL CONSTANT VECTORS INPUT  609
      IF(NB) 210,210,170                                                609
  170 IJ1 = 0                                                           609
      DO 200 K = 1,NB                                                   609
      DO 180 I = 1,NA                                                   609
      B1(I) = 0.0                                                       609
      IJ = I                                                            609
      DO 180 J = 1,NA                                                   609
      IJ2 = IJ1 + J                                                     609
      B1(I) = B1(I) + A(IJ) * B(IJ2)                                    609
  180 IJ = IJ + NAD                                                     609
      DO 190 I = 1,NA                                                   609
      IJ2 = IJ1 + I                                                     609
  190 B(IJ2) = B1(I)                                                    609
  200 IJ1 = IJ1 + NBD                                                   609
C                 SOLUTION VECTORS NOW IN B                             609
C                 CHECK FOR OVERFLOW CONDITION AND SET ERROR SIGNAL     609
  210 CALL OVERFL(INDEX)                                                609
      IF (INDEX-1)230,230,240                                           609
  230 IERROR = -1                                                       609
  240 RETURN                                                            609
C                 IF CONTROL REACHES 250, MATRIX IS SINGULAR OR A MACHINE 609
C                 ERROR HAS OCCURED                                     609
  250 IERROR = 1                                                        609
      GO TO 240                                                         609
      END                                                               609
```

III Sample Data Output

SAMPLE DATA OUTPUT

```
AMOUNT OF PROPELLANT, POUNDS
   LH2     =  7000.00
   RP-1    =  75300.00
   LO2     =  17700.00
   LF2     =  5000.00
EXPERIMENTAL VALUES OF T, P, V
DEGREES KELVIN  =  1800.0
ATMOSPHERES     =  1.0
CUBIC FEET      =  47000000.
```

THEORETICAL RESULTS

IDENTIFICATION OF PRODUCTS OF REACTION

H2O	CO2	H2	N2	F2
O2	HF	CO	NO	OH
H	N	F	C	O

47 ITERATIONS REQUIRED FOR SOLUTION

PARTIAL PRESSURES

0.000	0.000	0.439	0.278	0.
0.	0.013	0.202	0.000	0.000
0.000	0.000	0.000	0.068	0.000

POUND MOLES

0.00	0.00	8706.90	5512.21	0.
0.	263.16	4015.47	0.00	0.00
4.70	0.00	0.00	1353.13	0.00

PRESSURE, MOLE, VOLUME RATIOS

0.000	0.000	0.439	0.278	0.
0.	0.013	0.202	0.000	0.000
0.000	0.000	0.000	0.068	0.000

POUND WEIGHTS

0.	0.	17553.	154430.	0.
0.	5265.	112473.	0.	0.
5.	0.	0.	16251.	0.

WEIGHT RATIOS

0.0000	0.0000	0.0574	0.5047	0.
0.	0.0172	0.3676	0.0000	0.0000
0.0000	0.0000	0.0000	0.0531	0.0000

```
BURNING RATE, POUNDS
   LH2   =  7000.
   RP-1  =  75300.
   LO2   =  17700.
   LF2   =  5000.
AMOUNT OF ENTRAINED AIR
   MOLES  =  6960.

   POUNDS =  201599.
   PRESSURE, MOLE, VOLUME RATIO = 0.351
   WEIGHT RATIO = 0.6589

   TOTAL THEORETICAL POUND MOLES = 19856.

   THEORETICAL VOLUME = 46962371.
```

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